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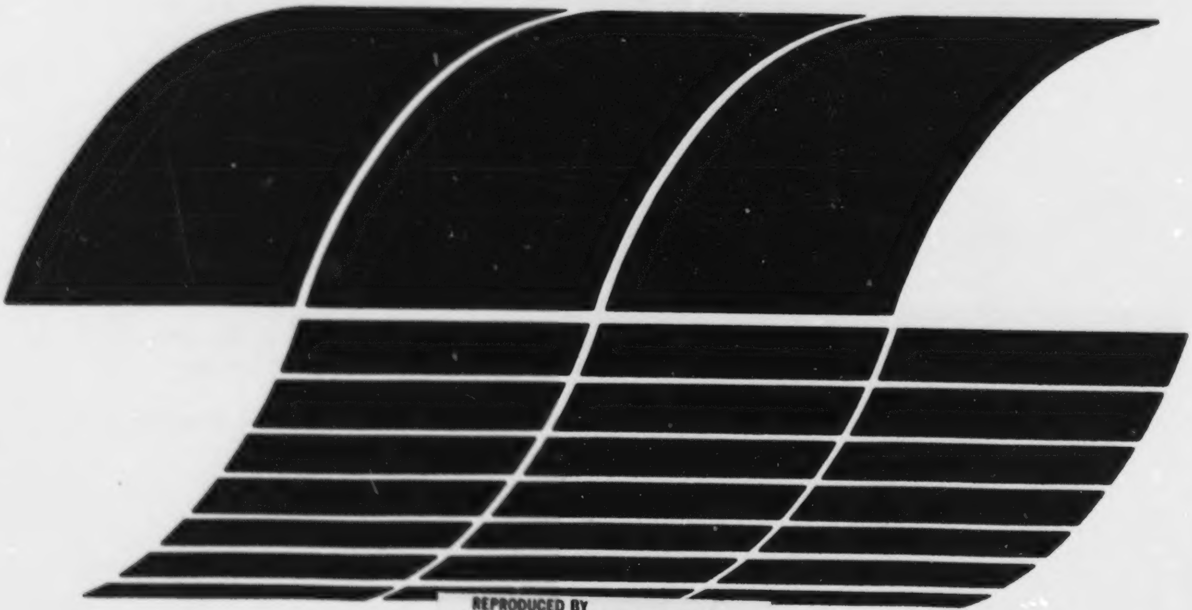

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16. ABSTRACT

The report gives results of a two-phased evaluation of Level 1 environmental assessment procedures. Results from Phase I, a field evaluation of the Source Assessment Sampling System (SASS), showed that the SASS train performed well within the desired factor of 3 Level 1 accuracy limit. Three sample runs were made with two SASS trains sampling simultaneously and from approximately the same sampling point in a horizontal duct. A Method-5 train was used to estimate the 'true' particulate loading. The sampling systems were upstream of the control devices to ensure collection of sufficient material for comparison of total particulate, particle size distribution, organic classes, and trace elements. Phase II consisted of providing each of three organizations with three types of control samples to challenge the spectrum of Level 1 analytical procedures: an artificial sample in methylene chloride, an artificial sample on a flyash matrix, and a real sample composed of the combined XAD-2 resin extracts from all Phase I runs. Phase II results showed that when the Level 1 analytical procedures are carefully applied, data of acceptable accuracy is obtained. Estimates of intralaboratory and interlaboratory precision are made.

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a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group	
Pollution	Chemical Analysis	Pollution Control	13B	07D
Assessments	Organic Compounds	Stationary Sources	14B	07C
Sampling	Particle Size	Environmental Assessment		
Analyzing				
Dust		SASS Train	11G	
Trace Elements		Particulate	06A,06P	

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Level 1 Environmental Assessment Performance Evaluation

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ABSTRACT

This report presents the results of a two-phased evaluation of Level 1 environmental assessment procedures. Phase I was a field evaluation of the Source Assessment Sampling System (SASS). Three sample tests were made with two SASS trains sampling simultaneously and from approximately the same sampling point in a horizontal duct. A Method 5 train was used to estimate the "true" particulate loading. The sampling systems were located upstream of the control devices to insure collection of sufficient material for comparison of total particulate, particle size distribution, organic classes, and trace elements. Phase II consisted of providing each of three participating organizations with three types of control samples to challenge the spectrum of Level 1 analytical procedures: an artificial sample in methylene chloride, an artificial sample on a flyash matrix, and a real sample composed of the combined XAD-2 resin extracts from all Phase I SASS runs. Estimates of intralaboratory and interlaboratory precision are made.

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ABBREVIATIONS

AA	Atomic Absorption
ADL	Arthur D. Little, Inc.
ANOVA	Analysis of Variance
CV	Coefficient of Variation
GC	Gas Chromatography
Grav	Gravimetric
HC	Hydrocarbon
IR	Infrared
LC	Liquid Chromatography
LRMS	Low Resolution Mass Spectroscopy
RTI	Research Triangle Institute
SASS	Source Assessment Sampling System
SDDC	Silver Diethyldithiocarbamate
SoRI	Southern Research Institute
SSMS	Spark Source Mass Spectrometry
TCO	Total Chromatographable Organics

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SECTION 1.0
INTRODUCTION

An experimental program designed to evaluate the source assessment sampling system (SASS) and the associated Level 1 analytical procedures has been completed. The project was conducted in two phases. Phase I consisted of a field evaluation of the SASS involving simultaneous sampling with two SASS trains and a Method 5 train. Results of Phase I are used to estimate within- and between-train precisions for particulate, organic, and inorganic sampling, and to estimate the biases of the SASS trains with respect to Method 5 for total particulate determinations. Phase II consisted of an interlaboratory evaluation of the analytical methods involving the analysis of split samples by participating laboratories.

The Research Triangle Institute (RTI) coordinated the experimental program with Arthur D. Little, Inc. (ADL), Southern Research Institute (SoRI), TRW, and Radian Corporation. ADL prepared all XAD-2 resin used in the field sampling; analyzed all the field samples collected in Phase I of the program; and prepared, analyzed, and distributed the control samples used in Phase II. SoRI and TRW each provided a field crew and a SASS train for Phase I and participated in Phase II by analyzing the control samples provided by ADL. Radian Corporation provided a field crew and a Method 5 train for Phase I and participated in Phase II by analyzing the control samples.

The objectives of this project were to evaluate both the SASS and the analytical procedures. Assessment of field crew and/or analyst performance was not a program objective. However, this study bears out the prediction that, with training, a good crew can learn to operate the SASS successfully. No major difficulties were encountered during the sampling phase. Actions taken to eliminate or minimize extraneous sources of variability in the field evaluation of the SASS included the following:

1. Each participating organization was requested to provide a crew experienced in the operation and field use of the SASS.
2. Field crews were briefed on and directed to use the approved and documented Level 1 sampling procedures (1).
3. RTI provided onsite coordination of the field sampling activities.
4. Calibration checks were made on the volume measurement systems (dry gas meters) of the SASS trains and on the gas velocity measurement systems of the two SASS trains and the Method 5 train.
5. All field samples were analyzed by one organization (i.e., ADL), eliminating the between-laboratory component of variability of the analytical methods.

In an effort to minimize analyst/laboratory biases in Phase II of the program, RTI personnel visited each organization to discuss the analytical procedures and to review the laboratory facilities and apparatus to be used in the analysis of the control samples. Also, as RTI analyzed the data for the final report, outliers or suspicious data were brought to the attention of the reporting organization for verification and/or correction as appropriate. For this test, laboratories were allowed to repeat calculations but were not allowed to repeat analysis.

A brief summary and interpretation of the results of both phases of the program are contained in Section 2.0 of this report. A description of the test plan for the field evaluation of the SASS and for the interlaboratory evaluation of the analytical procedures is given in Section 3.0. Results of the field evaluation of the SASS are presented and discussed in Section 4.0. The interlaboratory evaluation of the analytical procedures is described in Section 5.0.

SECTION 2.0
SUMMARY AND CONCLUSIONS

PHASE I: FIELD EVALUATION OF THE SASS

The SASS was evaluated under field conditions on a preselected, stable source characterized by high organics and high particulate loadings. Samples were collected with two SASS trains and a Method 5 train running simultaneously. Three complete sample tests were made, each test consisting of two SASS runs and a Method 5 run. The relative positions of the trains were fixed with the probes of the two SASS trains positioned at a point of average duct velocity and within a few inches of each other. The Method 5 train was positioned downstream from the SASS train and operated according to the Federal Register method; i.e., the duct was traversed, and isokinetic sampling conditions were maintained (3). To insure consistency, all analytical work for Phase I was done by one organization.

Particulate Loading and Sizing

For each SASS train run, the particulate on the filter and in each cyclone was dried and weighed to compare particle sizing between trains. The total particulate catches were then used to determine particulate loading for comparison to Method 5.

Results show the following:

1. Particle sizing compared very well between SASS's for the three tests.
2. Particulate concentrations determined by the SASS's compared very well with Method 5, the largest difference being within 20 percent.
3. The estimated precision between trains given as a standard deviation is 36 mg/m^3 (10 percent on a relative basis).

Collected Organics

A complete Level 1 organics analysis was carried out on the pair of SASS runs from Test 2. For this set, the organic material collected by the SASS's agreed well in quantity and composition (i.e., volatile, nonvolatile, and categories) and was collected proportionally in corresponding SASS components.

Collected Inorganics

For the same pair of SASS runs, mercury, arsenic, and antimony were determined on the combined second and third impingers by atomic absorption. For these limited analyses, the data for each element agree within a factor of two.

PHASE II: VERIFICATION OF THE LEVEL 1 ANALYTICAL PROCEDURES

Three aliquots of each of three sample types were supplied to each of the three participating organizations for analysis by current Level 1 procedures. The three sample types were:

1. A known, artificial, liquid sample containing 16 components.
2. A real particulate sample obtained from a source significantly different from the one selected for Phase I sampling.
3. The combined XAD-2 extracts from the SASS runs in Phase I.

A full Level 1 analysis was performed on one aliquot of each of the three sample types; the remaining aliquots were analyzed using a reduced Level 1 scheme.

Certain methods employed in the organic analysis scheme are still being refined, and interpretation of the organic data from complex sources can be an involved process requiring great attention to detail. However, from this preliminary analysis of Phase II data, it appears that the organic analysis scheme can yield results of adequate quality to satisfy Level 1 requirements provided that judicious care is exercised by the analyst to follow specified procedures and to utilize all the analytical data generated by the scheme in interpreting individual blocks of data.

Results of the inorganic sample preparation and SSMS analysis scheme indicate that, for some elements, variability in the analytical phase alone may be exceeding the allowable factor of 2 to 3 in the Level 1 procedures. It is expected that standardization of procedures among contractors will reduce this variability.

SECTION 3.0

DISCUSSION OF THE EXPERIMENTAL TEST PLAN

Procedures for Level 1 environmental assessments for both sample collection and sample analyses have been specified by the Process Measurements Branch (PMB) of the Industrial Environmental Research Laboratory (IERL) (1). In order for the Level 1 procedures to be effective, the precision and accuracy of both the sample collection and sample analysis phases of the measurement process must be sufficient to satisfy Level 1 data quality requirements.

The primary procedure for characterizing gaseous process streams in environmental assessments is to use the SASS for sample collection and specified analytical methods for subsequent sample analysis. The SASS and some of the analytical methods, at least for this application, are still in the developmental stage to the extent that prior to this study they had not been subjected to collaborative (or interlaboratory) tests. The purposes of this project were to evaluate the SASS under field conditions (Phase I) and to conduct an interlaboratory evaluation of the associated analytical methods (Phase II).

PHASE I: FIELD EVALUATION OF THE SASS

The SASS train evaluation test plan--starting with source selection criteria, continuing through sampling requirements, and ending with directions for sample analyses--is defined in the following paragraphs.

Source Selection Criteria

Criteria used in the source selection process were as follows:

1. The process stream should be sufficiently high in organics and particulate to provide a stiff challenge of the SASS train.
2. The process stream should be sufficiently stable to allow for comparison of data between days or tests.

3. The process stream must be amenable to this test in terms of space for simultaneous operation of two SASS trains and a Method 5 train, available electrical power to operate the trains and two mobile laboratories, and a physical stack or duct configuration such that sampling port locations for Method 5 are consistent with criteria set forth in EPA Reference Method 1 (2).

Examination of data from previous tests revealed a site which met the above conditions. The plant process was continual, the grain loading was 194.5 mg/m^3 (0.085 gr/ft^3) when sampling prior to the control device, and analysis of samples collected yielded significant concentrations of organic compounds.

Field Sampling

Samples were collected with the two SASS trains and the Method 5 train running simultaneously. Three complete sample tests were made. The relative positions of the trains were fixed with the probes of the two SASS trains positioned at a point of average duct velocity and within a few inches of each other. The Method 5 train was positioned downstream from the SASS train and operated according to the Federal Register method; i.e., the duct was traversed and isokinetic sampling conditions were maintained (3). The test site configuration is shown in Figure 1.

A calibration check of the dry gas meters showed the SASS's to agree within 3 percent on volume measurements. A comparison of the S-type pitot tubes on the SASS's against a standard pitot tube yielded coefficients of 0.84 and 0.89 as compared to the 0.85 ± 0.02 value assumed for well-manufactured S-type pitot tubes.

Analysis Scheme for Field Samples

To insure consistency, all analytical work for Phase I was done by one organization. Table 1 summarizes the analyses performed on the pair of SASS runs from one test. For the other two tests, the only analyses performed were gravimetric analyses of particulate for the cyclones, filter, and rinse. The analysis scheme of Phase I is described in the following listing.

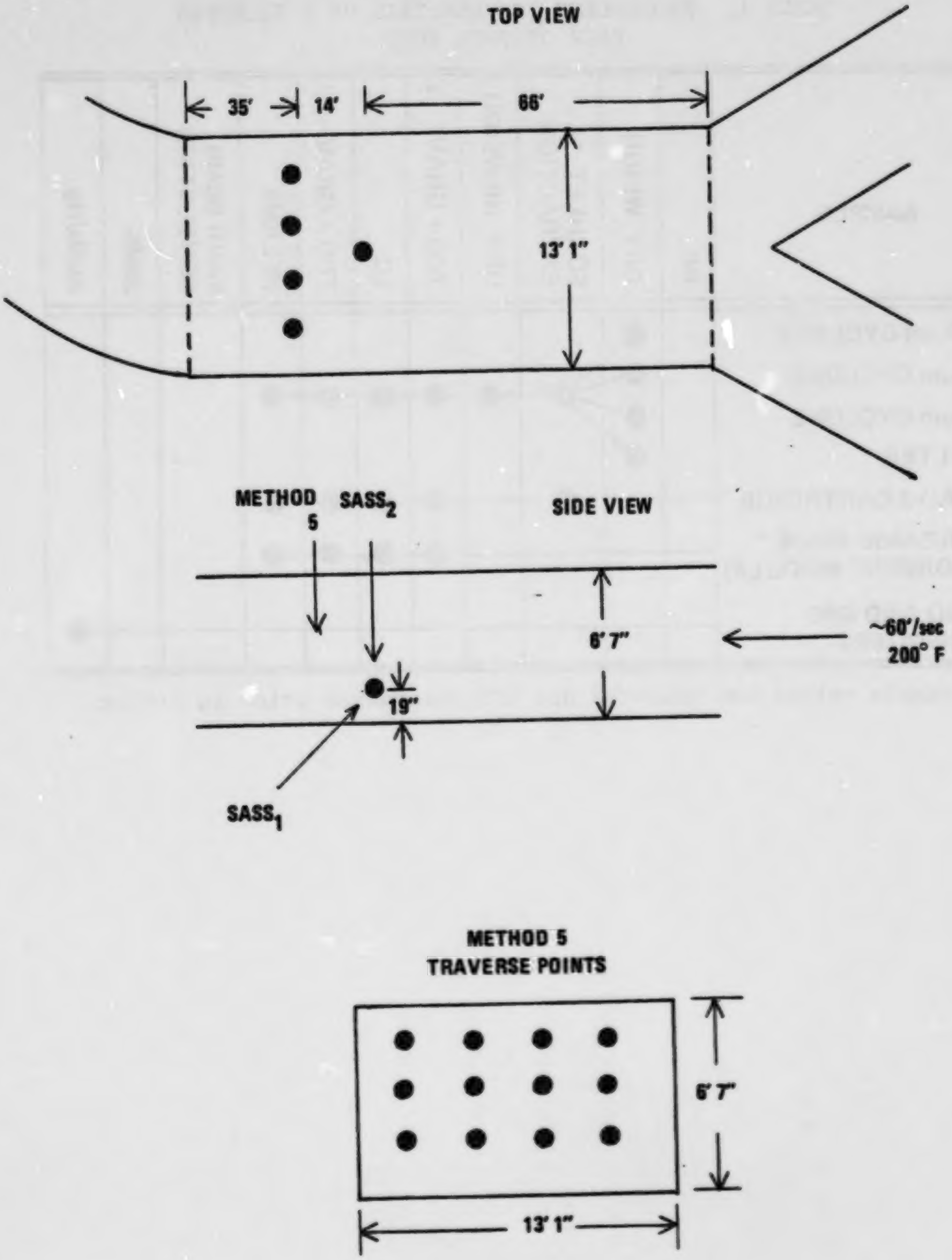

TOP VIEW
35'
14'
66'
13' 1"
METHOD 5
SASS$_2$
SIDE VIEW
6' 7"
~60'/sec
200° F
19"
SASS$_1$
METHOD 5
TRAVERSE POINTS
6' 7"
13' 1"

Figure 1. Test site configuration for field evaluation of the SASS.

TABLE 1. PROCEDURES FOR ANALYSIS OF A SELECTED PAIR OF SASS RUNS

SAMPLE	GC	DRY, WEIGH	SOXHLET EXTRACTION	DRY, RE-WEIGH	TCO + GRAV	LC	TCO + GRAV	IR-LRMS	PARR BOMB COMBUSTION	SSMS	As/Sb/Hg
10 μm CYCLONE		●									
3 μm CYCLONE		●	●	●	●	●	●	●			
1 μm CYCLONE		●									
FILTER		●									
XAD-2 CARTRIDGE			●		●	●	●	●			
ORGANIC RINSE* (SORBENT MODULE)					●	●	●	●			
2ND AND 3RD IMPINGERS											●

* Sample volume was measured and TCO determined prior to drying.

1. Particulate

   A. For each SASS train run, the particulate on the filter and in each cyclone was dried, then weighed, and the total weight of particulate determined. The particulate for each Method 5 run was also dried and weighed. Weighings were done in the field by one person. This allowed for a comparison of the SASS trains to each other and to the Method 5 for each test (same day) and on a day-to-day basis.

   B. For one test (two SASS trains and a Method 5 run simultaneously), the organics were extracted (soxhlet extraction) from the particulates and the particulates reweighed. The SASS particulate extracts were then analyzed for volatile (TCO) and nonvolatile (Grav) organic material and subjected to a full Level 1 organics analysis, including LC-IR-LRMS.

2. XAD-2 Module

   A. For each SASS run, the total weight (TCO + Grav) was to be determined for the condensate and for the combined XAD-2 extract and module rinse. However, the source yielded no condensate, and the extracts were inadvertently combined for Phase II before obtaining TCO and Grav data on the individual runs. In addition, the module rinses were not combined with the extracts from the XAD-2 module as specified in the original test plan since the methanol in the rinse solution would have interfered with class separation during LC fractionation. Instead, the rinses were evaporated separately to a tarry solid and introduced onto the silica surface.

   B. On the same pair of runs selected for the particulate organic analysis, the above TCO + Grav determinations were followed by eight class separations with a TCO + Grav determination on each of the fractions. The fractions were also analyzed by the IR-LRMS scheme.

3. Impingers

   For the same pair of runs selected for particulate organics analysis and XAD-2 eight class separation, Hg, As, and Sb were determined on the combined second and third impingers by current Level 1 methods. No analyses were done on the impinger solutions for the remaining tests.

PHASE II: VERIFICATION OF THE ANALYTICAL SCHEME

Three aliquots of each of three sample types were supplied to each of the three participating organizations for analysis by current Level 1 procedures. The three sample types were as follows:

1. A known, artificial, liquid sample containing 16 components; the three aliquots were not identical but contained different amounts of certain components;
2. A real particulate sample obtained from a source significantly different from the one selected for Phase I sampling; the three aliquots were identical;
3. The combined XAD-2 extracts from all the SASS runs in Phase I; the three aliquots were identical.

The samples were coded and specific instructions for the analytical work to be done on each were provided. Each participant did a full Level 1 analysis on one aliquot of each of the above three sample types. For the other two aliquots of each type, there was a reduced analysis scheme.

Analysis Scheme for Control Samples

Procedures for analysis of the control samples for Phase II of the evaluation are summarized in Table 2 and discussed in the following paragraphs.

1. Sample 1
   - A. Aliquot 1. This aliquot was taken through a complete Level 1 organic analysis beginning with a TCO + Grav. The sample was then separated into eight fractions by LC with a TCO + Grav and IR-LRMS on each fraction.
   - B. Aliquot 2 and 3. The analysis of these aliquots involved a TCO + Grav, eight class separation by LC, and TCO + Grav on each of the eight fractions.

TABLE 2. PROCEDURES FOR ANALYSIS OF PHASE II SAMPLES

	SOXHLET EXTRACTION	TCO + GRAV	LC	TCO + GRAV	IR-LRMS	PARR BOMB COMBUSTION	SSMS PLUS As/Hg/Sb
SAMPLE 1							
ALIQUOT 1		●	●	●	●		
ALIQUOTS 2 AND 3		●	●	●			
SAMPLE 2							
ALIQUOT 1	●	●	●	●	●	●	●
ALIQUOT 2 AND 3	●	●					
SAMPLE 3							
ALIQUOT 1		●	●	●	●		
ALIQUOT 2 AND 3		●					

2. Sample 2
    A. Aliquot 1. The analysis of this sample type followed the Level 1 scheme for particulates. One portion of the sample was extracted and a TCO + Grav performed on the extract. The extract was then separated into eight fractions by LC and a TCO + Grav and IR-LRMS performed on each fraction. The remaining particulate was Parr-bomb combusted and analyzed by SSMS and by approved Level 1 procedures for As/Hg/Sb.
    B. Aliquot 2 and 3. These two aliquots were extracted and a TCO + Grav performed on the extract.
3. Sample 3
    A. Aliquot 1. Analysis of this combined extract sample started with a TCO + Grav followed by the eight class LC separation with a TCO + Grav and IR-LRMS on each of the eight fractions.
    B. Aliquots 2 and 3. These two aliquots involved only a TCO + Grav analysis.

Composition of Artificial Control Samples

The compositions of the artificial samples in methylene chloride and the artificial sample on a flyash matrix are given in Appendix A. During the analysis phase these compositions were known only to ADL, RTI, and EPA.

SECTION 4.0
RESULTS OF SASS EVALUATION

The purpose of an interlaboratory test is, within the project constraints, to do the following:

1. Where possible, compare the experimental system results with reference methods or standard material (accuracy).
2. Compare results between similar sets of equipment operated by different laboratories (reproducibility and interlaboratory precision).
3. Compare duplicate results from the same system operated by the same laboratory (repeatability or intralaboratory precision).

Measurements for which data are available and the order in which they will be discussed are as follows:

1. Particulate concentration determinations allowing comparison of the SASS's with Method 5 and with each other for three tests.
2. Particle size fractionation between SASS's for three tests.
3. Total (volatile and nonvolatile) organics by LC fractions between SASS's for one test.
4. Organic categories in samples between SASS's for one test.
5. IR results (functional groups) for samples between SASS's.
6. Categories, subcategories, and specific compounds identified by LRMS between SASS's.
7. Organic material collected between SASS's for one test.
8. Arsenic, mercury, and antimony determinations for one sample between SASS's.

PARTICULATE CONCENTRATIONS DETERMINATION

Three complete tests were made with the two SASS's and the Method 5 train sampling simultaneously as described in the test plan discussion. This experiment was designed so that the results could be analyzed by analysis-of-variance (ANOVA) methods. Particulate concentration determinations are given by train and by test number in Table 3. The corresponding ANOVA table is shown as Table 4.

Basically, the ANOVA is an analysis of differences in means based on the fact that if the means of subgroups differ significantly, the variance of the combined groups is much larger than the variances of the separate groups (ref. 4). For this experiment, a two-way classification ANOVA is used wherein the variation among trains and the variation among tests are estimated and individually compared to the estimated experimental error (residuals in Table 4). The objectives of this analysis are to test the following hypotheses:

1. Hypothesis 1: There are no differences between trains.
2. Hypothesis 2: There are no differences between tests.

If the first (second) hypothesis is true, then from Table 4

$$F_t = \frac{\sigma^2 + 3\sigma_t^2}{\sigma^2} \qquad \left(F_r = \frac{\sigma^2 + 3\sigma_r^2}{\sigma^2}\right)$$

is a value of a random variable having the F distribution with t-1=2 (r-1=2) degrees of freedom (df) and (t-1) (r-1) = 4 degrees of freedom. Thus, if the calculated F value is less than the tabulated F value for 2 and 4 degrees of freedom at the selected $\alpha = 0.05$ level of significance, this hypothesis cannot be rejected for that level of significance.

The calculated values of F_r and F_t are 0.25 and 2.96, respectively. The tabulated value of F for 2 and 4 degrees of freedom at the 0.05 level of significance is 6.94. Therefore, both of the previously stated hypotheses must be accepted at the 95% confidence limit.

In essence, the above analysis shows that the variability among trains (or among tests) is no greater than what would be expected from experimental error alone.

From the ANOVA, the best estimate of the precision of a single observation, regardless of train (intertrain precision), is

$$(\sigma^2 + \sigma_t^2)^{\frac{1}{2}} = 36 \text{ mg/m}^3$$

The coefficient of variation (or relative standard deviation) is 0.10, or 10 percent. Intratrain precision is estimated by σ and is equal to 28 mg/m.^{3}

TABLE 3. PARTICULATE CONCENTRATION mg/m^3

Test #	SASS 1	SASS 2	M 5	Train Total
Test 1	408	337	342	1,087
Test 2	399	349	322	1,070
Test 3	353	315	371	1,039
Total	1,160	1,001	1,035	3,196

σ = 28 mg/m^3 (8%) WITHIN TRAIN PRECISION.

$(\sigma^2 + \sigma_t^2)^{1/2}$ = 36 mg/m^3 (10%) BETWEEN TRAIN PRECISION.

TABLE 4. ANALYSIS OF VARIANCE TABLE

Source	Sum of squares	Degrees of freedom	Mean square	Estimate of
Tests	395	2	197	$\sigma^2 + 3\sigma_r^2$
Trains	4,674	2	2,337	$\sigma^2 + 3\sigma_t^2$
Residual	3,154	4	789	σ^2
Total	8,223	8		

For between tests, the component of variance given by σ_r^2 as calculated from Table 4 resulted in a negative value. That variance component is then assumed to be zero or very small compared to experimental error; i.e., $\sigma_r \ll \sigma$.

The results of this evaluation indicate that SASS's precision and accuracy were not significantly different from the precision and accuracy of the Method 5 determinations.

PARTICLE SIZE FRACTIONATION

Particle matter is divided into four size fractions by the SASS using three cyclones and a filter in series. From Table 3, comparison of particulate concentration measurements can be made. The particulate concentration, as determined from each cyclone and the filter, is given as a percent of the total concentration determined by the train in Figure 2. As seen from the figure, results from corresponding components of the SASS's compare very well for all tests.

ORGANIC EXTRACTABLES

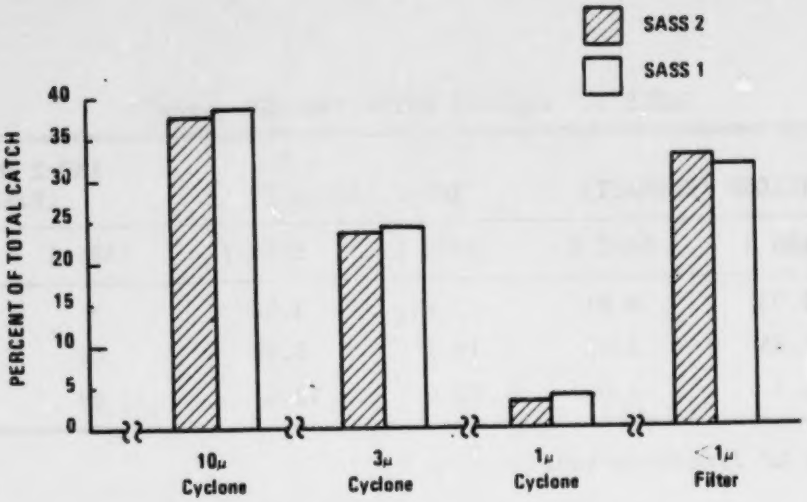
Extracting organic matter from SASS samples is an important procedure in the analysis process. Table 5 compares the volatile (TCO) and nonvolatile (Grav) organic contents of the samples taken from corresponding components of the SASS's. The data show that organic material collected by the corresponding components was comparable in quantity (total) and in composition (volatile and nonvolatile).

ORGANICS IN LC FRACTIONS

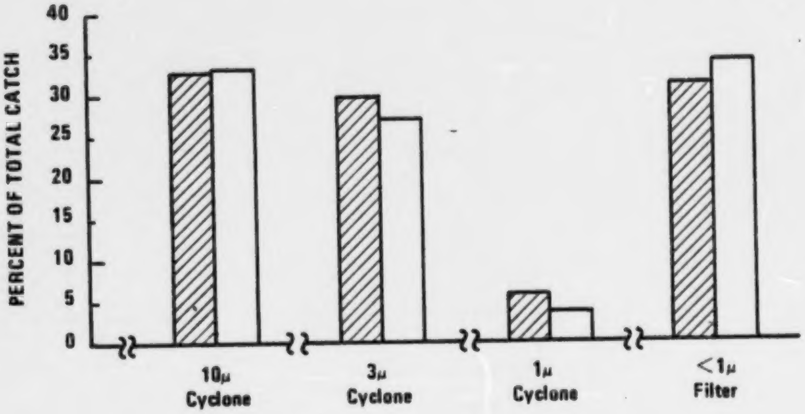
In the Level 1 analysis procedures, the sample extract is separated by silica gel liquid chromatography and a solvent gradient series into 8 fractions of varying polarity. TCO and gravimetric analyses of each fraction are done to determine the distribution of the sample by the various class types.

Comparison of the distribution of the samples in terms of volatile and nonvolatile organics by LC fractions is given in Table 6.

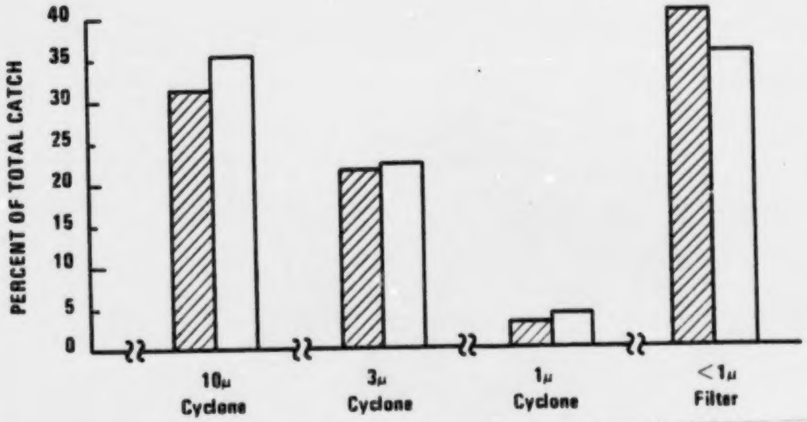
As seen from the table, the totals (Σ) across all fractions for TCO and Grav agree very well. The comparison for individual fractions with few exceptions is good.



COMPARISON OF PARTICLE SIZE FRACTIONATION (Test 1)



COMPARISON OF PARTICLE SIZE FRACTIONATION (Test 2)



COMPARISON OF PARTICLE SIZE FRACTIONATION (Test 3)

Figure 2. Comparison of particle size fractionation of two SASS's.

TABLE 5. ORGANIC EXTRACTABLES* (mg/m^3)

	CYCLONE (EXTRACT)		XAD-2 (EXTRACT)		XAD-2 MODULE (RINSE)	
	SASS 1	SASS 2	SASS 1	SASS 2	SASS 1	SASS 2
TCO	0.03	0.01	3.41	3.58	–	–
GRAV	1.65	1.58	10.2	8.99	69	81
TOTAL	1.7	1.6	13.6	12.6	69	81

*Totals after LC fractionation.

TABLE 6. ORGANIC EXTRACTS SUMMARY
(SASS 1/SASS 2)

Cyclone Extract

	LC 1	LC 2	LC 3	LC 4	LC 5	LC 6	LC 7	LC 8	Σ
Total Organics mg/m^3	0.03	<0.01	0.54	0.22	0.10	0.68	<0.01	0.10	1.7
	0.01	0	0.61	0.15	0.06	0.73	0.01	0	1.6
TCO, mg	0.8	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	1.0
	0.2	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.5
Grav, mg	0	0	16.8	6.8	3.2	21.2	0	3.2	51
	0	0	19.2	4.8	2.0	23.2	0.4	0	50

XAD-2 Extract

	LC 1	LC 2	LC 3	LC 4	LC 5	LC 6	LC 7	LC 8	Σ
Total Organics mg/m^3	0.54	0.71	8.1	0.95	0.35	1.5	0.47	0.01	12.6
	0.33	2.4	8.8	0.59	0.25	0.93	0.24	0.07	13.6
TCO, mg	5.2	19	73	6.7	3.7	5.3	0.1	0.2	113
	2.6	35	58	1.7	1.1	5.7	0.1	2.1	106
Grav, mg	13	3.3	182	23	7.3	41	15	0	284
	7.5	38	216	17	6.7	23	7.3	0	315

Sorbent Module Rinse

	LC 1	LC 2	LC 3	LC 4	LC 5	LC 6	LC 7	LC 8	Σ
Total Organics mg/m^3	1.6	1.3	8.9	19.7	12.9	9.9	14.6	0	69
	1.6	1.3	14.4	28.5	6.6	8.5	16.9	3.1	81
	-	-	-	-	-	-	-	-	-
Grav, mg	49.9	39.5	277	612	400	306	454	0	2,138
	51.7	41.4	455	900	207	269	533	98.2	2,555

FUNCTIONAL GROUPS IDENTIFIED BY IR

IR spectroscopy is used in the Level 1 environmental assessment procedures to determine the types of functional groups present in a sample. Table 7 compares the results of the IR analyses of the samples before LC separation. The band position ($\bar{\nu}$, cm^{-1}), intensity [weak (W), medium (M), or strong (S)], and functional group assignments are indicated. Agreement is good between samples taken from corresponding components of the two SASS trains. Bands identified in only one of the two samples are of weak intensity. The IR results for the LC fractions of the samples are given in Appendix B.

CATEGORIES, SUBCATEGORIES, AND SPECIFIC COMPOUNDS IDENTIFIED BY LRMS

A low resolution mass spectrum (LRMS) is obtained on all LC fractions that exceed the concentration threshold (TCO + Grav $\geq$ 0.5 mg/m^3) in order to determine the principle compound types present in each fraction.

Interpretation of the LRMS spectra is guided by knowledge of the LC separation scheme and information from the IR spectra. When results are reported, increasingly more specific data are presented as the complexity or simplicity of the spectra will allow. The first level of reporting is identification of compound classes. Appendix C compares the categories identified in the organic extracts of samples taken from corresponding components of SASS 1 and SASS 2. Molecular weight range and composition are estimated with ratings of 100 = major, 10 = minor, and 1 = trace. The more specific data (subcategories and compounds) are reported in Appendix D.

ORGANIC CATEGORIES SUMMARY

Identification and quantification of organic categories in process streams are the ultimate goals of a Level 1 organics analysis. Table 8 lists the categories and their concentrations for one set of SASS runs as determined by the combination of all organic analytical methods (i.e., TCO + Grav, IR, and LRMS). As seen in the table, the categories compare well across trains, both qualitatively and quantitatively.

Qualitatively, only inorganics at 0.1 mg/m^3 and silicones at 0.1 mg/m^3 were identified in the SASS 1 sample and not the SASS 2 sample. Quantitatively, when the concentration levels are considered, only the difference in the heterocyclic O concentrations appears to be much larger than desired.

TABLE 7. FUNCTIONAL GROUPS IN SASS SAMPLES IDENTIFIED BY IR (BEFORE LC SEPARATION)

a. Cyclone Extracts SASS 1			SASS 2		
$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
3,050	M	aromatic CH	3,050	M	unsaturated CH
2,950, 2,920, 2,850	M	aliphatic CH	2,920	M	saturated CH
			1,920	W	allene, $C=C=CH_2$
1,720	S	imide, carbamate, lactone, dialkyl ketone, α-Cℓ ketone	1,710	M	imide, carbamate, dialkyl ketone, ester
			1,660	M	ketone, C=N, C=C
1,600	M	ring vibrations	1,600	M	aromatic ring
1,450	M	CH_2, CH_3	1,450	M	CH_2, aromatic CH, CH_3
1,380	W	CH_3, $SiCH=CH_2$			
1,280	M	$SiCH_3$, $C-O-NO_2$			
			1,250	M (broad)	ester, ether
810	M	$SiCH_3$, substituted pyridine	810	M	substituted pyridine, substituted aromatic, C=CH, fused ring compound
750	S	aromatic, fused rings	750	S	aromatic, fused rings, substituted pyridine
b. XAD-2 Extracts					
3,400	VW (broad)	NH, OH	3,400	W (broad)	OH, NH
3,050	M	aromatic CH	3,050	M	aromatic CH
2,950-2,930	M	aliphatic CH	2,950-2,930	M	aliphatic CH
1,700	W	ester, amide, ketone, unsubstituted amidine HCℓ, carbamate, imide,	1,700	W	ester, amide, ketone, unsubstituted amidine HCℓ, carbamate, imide
1,600	M	C-N=O, N-C=N, ring vibrations	1,600	M	C-N=O, N-C=N, ring vibrations

(continued)

TABLE 7 (continued)

b. XAD-2 Extracts (con.) SASS 1			SASS 2		
$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
1,500	W	ring vibrations	1,500	W	ring vibrations
1,460-1,420	M	Si-aromatic, SCH_2-, 3-substituted pyridine, aliphatic and aromatic CH, $SiCH_2$-	1,460-1420	M	phenyl-Si, S-CH_2-, 3-substituted pyridine, aliphatic and aromatic CH, Si-CH_2-
1,180	M	ester, SiO-CH_3, $C_3P=O$	1,180	M	ester, SiO-CH_3, $C_3P=O$
850-700	S(multiple)	substituted aromatic or fused rings	850-700	S(multiple)	substituted aromatic, fused rings
c. Sorbent Module Rinses					
			3,400	W	OH, NH
3,050	M	unsaturated CH	3,050	M	unsaturated CH
2,920	W	saturated CH	2,920	W	saturated CH
1,615, 1,600	M	ring vibrations, C=C, N-C=N	1,620	M	C=C, N-C=N
			1,600	M	aromatic ring
1,460, 1,450, 1,440 1,430	M	CH_2, CH_3, CH_3 aromatic, $CH_2C\ell$, SCH_3, SCH_2	1,460-1,430	M(multiplets)	CH_2, CH_3, $CH_2C\ell$ SCH_3, SCH_2
1,380	W	CH_3	1,380	W	CH_3
1,300	V	S-CH_3	1,300	VW	S-CH_3
1,260	W	$CH_2C\ell$	1,260	W	$CH_2C\ell$
1,240	W	S-CH_2	1,240	W	S-CH_2
840-700	S(multiple)	aromatic, fused rings	840-700	S(multiplets)	aromatic ring, fused rings, substituted pyridine
740	S	C-$C\ell$	740	S	C-$C\ell$

TABLE 8. ORGANIC CATEGORIES IN SASS SAMPLES

Categories	Concentration(mg/m^3) SASS 1	 SASS 2
Aliphatic hydrocarbons	1.1	1.1
Halogenated aromatic HC's	-	-
Aromatic HC's-benzene	0.6	0.1
<216	28.7	28.2
>216	25.6	28.7
Heterocyclic N	20.1	24.0
Heterocyclic S	2.4	2.5
Heterocyclic O	2.2	6.7
Phenols	0.2	0.3
Esters	0.5	0.2
Ethers	-	-
Amines	-	-
Amides	-	-
Carboxylic acids	0.6	0.7
Sulfonic acids, sulfoxides	-	-
Sulfur	0.2	0.7
Inorganics	0.1	-
Unclassified	0.3	1
Silicones	0.1	-

ARSENIC, MERCURY, AND ANTIMONY COMPARISONS

Arsenic, mercury, and antimony are determined by atomic absorption in the Level 1 procedures. Table 9 compared the levels of these elements found in the impinger solutions from the two SASS's. The estimates of precision of analysis were provided by Arthur D. Little, Inc. The agreement appears reasonable, based on the precision estimates for As and Sb. However, the difference in the Hg concentrations, although less than a factor of two, is larger than would be expected from analysis imprecision alone.

TABLE 9. ARSENIC, MERCURY AND ANTIMONY DETERMINATIONS

	As ($\mu g/m^3$)	Hg ($\mu g/m^3$)	Sb ($\mu g/m^3$)
SASS 1	0.83	0.40	0.10
SASS 2	0.71	0.24	0.06

ESTIMATED PRECISION OF ANALYSIS
CV(As) = 5%, CV(Hg) = 10%, CV(Sb) = 25%

SECTION 5.0
RESULTS OF ANALYTICAL METHODS EVALUATION

Evaluation of Level 1 environmental assessment methodologies for analysis of SASS samples was performed by providing control samples of three types to the participating laboratories. The control samples were prepared and analyzed by Arthur D. Little, Inc. Arthur D. Little's results are used as a fourth set of data for interlaboratory comparisons. Laboratories or participants are coded as A, B, C, and D and are not further identified in this report.

ORGANIC ANALYSIS RESULTS

The order of discussion for organic analyses follows the analytical scheme presented in Table 2. That order is:

1. TCO + Grav analyses of each of the three samples types.
2. TCO + Grav analyses of the LC fractions.
3. IR analyses of LC fractions.
4. LRMS analyses of LC fractions.

TCO and Grav Analyses of Phase II Samples

The first step in analyzing a Level 1 sample is the determination of the volatile (TCO) and nonvolatile (Grav) organic contents in the sample. Tables 10-12 compare the initial TCO and Grav values determined by the four participants for three aliquots of each of the three sample types. The three aliquots of the artificial sample in methylene chloride were not identical and yield interlaboratory comparisons only. However, the aliquots of the artificial sample on a flyash matrix and of the field sample were identical and may be compared for intralaboratory repeatability as well.

XAD-2 Extract Results--

Total organic (TCO + Grav) determinations for the field sample (Table 13) show good agreement. The average and coefficient of variation (CV) of the 12 determinations are 480 mg and 4 percent, respectively. The range for the 12 values is only 52 mg or 11 percent of the average.

TABLE 10. TCO/GRAV RESULTS: ARTIFICIAL SAMPLE IN CH_2Cl_2 (mg)

		TCO		GRAV		TOTAL	
Aliquot 1	A	106		121		227	
	B	100		171		271	
	C	105	AVG = 97	167	AVG = 126	272	AVG = 222
	D	76	CV = 15%	44	CV = 47%	120	CV = 32%
Aliquot 2	A	97		104		201	
	B	79		146		225	
	C	92	AVG = 99	129	AVG = 108	221	AVG = 207
	D	129	CV = 21%	51	CV = 39%	180	CV = 10%
Aliquot 3	A	143		169		312	
	B	106		213		319	
	C	132	AVG = 159	248	AVG = 183	380	AVG = 342
	D	256	CV = 42%	100	CV = 35%	356	CV = 9%

Known weights of organics:

Aliquot 1 - 246.1 mg/20 ml
Aliquot 2 - 192.0 mg/20 ml
Aliquot 3 - 302.6 mg/20 ml

TABLE 11. TCO/GRAV RESULTS: ARTIFICIAL SAMPLE ON FLYASH MATRIX (mg)

		TCO	GRAV	TOTAL
Aliquot 1	A	71.2	67.6	139
	B	69	104	173
	C	144	69	213
	D	51	47	98
Aliquot 2	A	70.3	72.0	142
	B	81	124	205
	C	97	62	159
	D	12 mg/g	12 mg/g	
Aliquot 3	A	62.5	73.0	136
	B	82	135	217
	C	314	51	365
	D	12 mg/g	14 mg/g	

	TCO	GRAV	TOTAL
	AVG = 104 CV = 75%	AVG = 80 CV = 37%	AVG = 185 CV = 40%

TABLE 12. TCO/GRAV RESULTS: FIELD SAMPLE, XAD-2 EXTRACT (mg)

		TCO	GRAV	TOTAL
Aliquot 1	A	106	386	492
	B	78	380	458
	C	88	359	447
	D	150	340	490
Aliquot 2	A	144	343	487
	B	64	432	496
	C	110	366	476
	D	86	360	446
Aliquot 3	A	142	354	496
	B	46	428	474
	C	118	380	498
	D	134	360	494
		AVG = 106 CV = 32%	AVG = 374 CV = 8%	AVG = 480 CV = 4%

Determinations of nonvolatile organics showed good interlaboratory agreement. The average and CV for the 12 values are 374 mg and 8 percent, respectively.

TCO determinations show within laboratory CV's of 16, 26, 15, and 27 percent for participants A, B, C, and D, respectively. The agreement between participants A, C, and D is good. Participant B reports an average value of 63 mg, almost half of what the other participants reported.

Examination of the TCO procedures used revealed that participant B was operating the GC at a lower injection port temperature than the other participants were. This may account in part for the lower TCO values reported. Participant B also interpreted the Grav procedure as being a single weight. The samples were not taken to dryness, which would account for higher Grav values. The combination of low TCO's and high Grav's resulted in totals which were comparable to those of the other laboratories.

Artificial Sample Results--

The artificial samples show greater variation in both the individual TCO and Grav values and in the totals. Averages and coefficients of variation are indicated in the tables. In addition, Table 10 for the artificial sample in methylene chloride gives the known weight of organics for each of the three aliquots. For this sample, the total (TCO + Grav) weights obtained by the laboratories are well within the accuracy limits of Level 1.

TCO and Grav Analyses of the LC Fractions

Results of the TCO and Grav analyses of the LC fractions for the three sample types are given in Tables 13-17. The data show an overlap or "smearing" of fractions, resulting in differences in distribution among the four contractors. For example, the totals (TCO + Grav) for fraction 2 and for fraction 3 of the XAD-2 extract (Table 17) show large differences among the four contractors, whereas the sums of fractions 2 and 3 are fairly consistent.

Observation of the low total Grav value for Lab D as compared to the other labs and the theoretical total (216 mg) indicates quite different drying procedures or incomplete stripping of the column. However, the distribution of TCO values across all LC fractions for Lab D points more strongly to a drying problem than to column problems. Apparently, more detailed and specific procedures would improve comparability among labora-

TABLE 13. TCO/GRAV RESULTS: ARTIFICIAL SAMPLE IN CH_2Cl_2, ALIQUOT 1 (mg)

	TCO				GRAV				TOTAL			
	A	B	C	D	A	B	C	D	A	B	C	D
LC1	14.0	2.6	23.3	14	19.3	14.7	11.4	---	33	17	35	14
LC2	15.3	<0.30	10.0	10	0	1.0	9.0	---	15	<1	19	10
LC3	24.6	9.6	17.2	5.4	22.0	45.2	19.6	---	47	55	37	5
LC4	12.7	2.8	7.4	3.1	3.3	13.0	19.4	---	16	16	27	3
LC5	11.3	1.6	2.9	2.4	20.0	18.7	1.2	---	31	20	4	2
LC6	44.3	7.6	28.0	18.0	93.9	65.1	60.7	8	138	73	89	26
LC7	0.3	0.21	9.4	----	0	24.3	0	---	0	25	9	--
LC8	3.0	<0.30	N.R.	4.5	12.0	15.8	0	---	15	16	0	5
TOTAL	125.5	25.0	98.2	57.4	170.5	197.8	121.3	8	295	223	220	65

*Very low (0.1 mg) gravimetric values that fluctuated with time were not reported by Lab D.

TABLE 14. TCO/GRAV RESULTS: ARTIFICIAL SAMPLE IN CH_2Cl_2, ALIQUOT 2 (mg)

	TCO				GRAV				TOTAL			
	A	B	C	D	A	B	C	D	A	B	C	D
LC1	12.0	7.5	69.6	10	19.3	16.1	12.6	---*	31	24	82	10
LC2	18.0	<0.30	17.3	19	8.0	1.7	11.3	4.4	26	<2	29	23
LC3	22.6	10	21.4	17	24.0	42	10.3	---	47	52	32	17
LC4	17.0	4.1	7.6	11	4.0	11.6	10.0	---	21	16	18	11
LC5	4.7	1.0	17.8	4.0	10.0	6.6	0.5	---	15	8	18	4.0
LC6	42.6	5.0	26.1	36	38.0	40	35.9	31	81	45	62	67
LC7	2.0	<0.30	6.8	--	0	15.8	0	4.4	2	16	7	4.4
LC8	9.3	<0.30	N.R.	3.1	5.3	16.6	0	77	15	17	0	80
TOTAL	128.2	28.5	166.6	100.1	108.6	150.4	80.6	116.8	238	180	248	216

*Very low (0.1 mg) gravimetric values that fluctuated with time were not reported by Lab D.

TABLE 15. TCO/GRAV RESULTS: ARTIFICIAL SAMPLE IN CH_2Cl_2, ALIQUOT 3 (mg)

	TCO				GRAV				TOTAL			
	A	B	C	D	A	B	C	D	A	B	C	D
LC1	20.6	9.4	42.7	39	17.6	11.6	8.1	---*	38	21	51	39
LC2	10.3	<0.30	6.4	24	4.0	3.8	2.7	---	14	4	9	24
LC3	24.6	3.4	31.6	15	24.0	41	30.6	---	49	44	62	15
LC4	28.0	1.9	15.5	18	26.0	18.1	42.7	20	54	20	58	38
LC5	11.0	2.3	1.3	2.3	22.6	31.2	1.3	---	34	34	3	2
LC6	47.0	11	68.3	56	79.9	91	93.5	52	127	102	162	108
LC7	2.7	0.63	36.3	1.2	10.0	69	0	40	13	70	36	41
LC8	0	<0.30	N.R.	12	5.3	15.6	0	24	5	16	0	36
TOTAL	144.2	29.2	202.1	167.5	189.4	281.3	179	136	334	311	381	303

*Very low (0.1 mg) gravimetric values that fluctuated with time were not reported by Lab D.

TABLE 16. TCO/GRAV RESULTS: ARTIFICIAL SAMPLE ON FLYASH MATRIX, ALIQUOT 1 (mg)

	TCO				GRAV				TOTAL			
	A	B	C	D	A	B	C	D	A	B	C	D
LC1	12.3	9.4	4.9	12	21.0	40	6.5	---*	33	49	11	12
LC2	7.7	1.6	3.4	20	4.0	4.0	2.3	---	12	6	6	20
LC3	14.0	3.8	2.6	1.1	18.6	26	9.9	---	33	30	12	1
LC4	1.7	<0.20	0.3	1.5	8.7	8.2	9.3	---	10	8	10	2
LC5	0.1	<0.20	2.6	0.13	8.7	4.8	4.4	---	9	5	7	0
LC6	21.3	15	11.9	1.1	18.6	30	6.7	6.7	40	45	19	8
LC7	0.7	3.4	7.0	0.73	2.7	6.8	0	0.45	3	10	7	1
LC8	0	<0.20	N.R.	24	10.7	8.2	0	4.4	11	8	0	28
TOTAL	57.8	33.8	32.7	60.6	93.0	128.0	39.1	11.6	151	161	72	72

*Very low (0.1 mg) gravimetric values that fluctuated with time were not reported by Lab D.

TABLE 17. TCO/GRAV RESULTS: FIELD SAMPLE, XAD-2 EXTRACT, RUN 1 (mg)

	TCO				GRAV				TOTAL			
	A	B	C	D	A	B	C	D	A	B	C	D
LC1	1.4	<0.4	12.0	2.1	11.5	4.0	4.8	---*	13	4	17	2
LC2	15.2	<0.4	60.3	120	4.6	6.4	84.2	200	20	7	145	320
LC3	54.7	31	40.3	2.6	259.4	284	177.6	19	314	315	218	22
LC4	0.5	2.3	9.2	1.4	10.1	22	12.8	---	11	24	22	1
LC5	0.9	0.84	0.4	7.4	31.3	8.8	7.6	---	32	10	8	7
LC6	3.2	1.0	18.4	13	16.6	38	27.1	110	20	39	46	123
LC7	0.5	<0.4	21.6	1.9	2.8	23	3.6	---	3	23	25	2
LC8	0.9	<0.4	N.R.	8.3	3.7	37	0	50	5	37	0	58
TOTAL	77.3	36.7	162.2	156.7	340	423.2	317.7	379	418	459	481	535

*Very low (0.1 mg) gravimetric values that fluctuated with time were not reported by Lab D.

tories. Such procedures are included in the revised Level 1 Procedures Manual.

Identification of Functional Groups by IR

Two sets of IR data are presented for each sample type. One set is presented in Tables 18-20 and represents a listing of the functional groups identified by three participants in each of the sample types prior to LC separation. (Lab C did not include total sample IR spectra in the first report; these data were received later and are included in Appendix H). The other set of data, given in Appendix E, graphically represent IR results by LC fraction and participants. Intensity of an IR peak is indicated by the length of the line, and broad bands are indicated by a horizontal line of appropriate width. Listings of functional groups identified in each of the LC fractions are given in Appendix F.

In view of the complexity of the samples before LC fractionation, it is not surprising that there is not a one-to-one correspondence of spectra in Tables 18-20. In most cases where a band is identified by only one lab, the band is of medium or weak intensity.

Examination of the data presented in Appendix E reveals the same type of fractional overlaps as were noted in the TCO and Grav analyses. In addition, Laboratories C and D reported a number of bands that are not reported by Laboratory A or B. Possible explanations are sample contamination, artifacts from the column, or sensitivity of the IR spectrometer used.

Categories, Subcategories, and Specific Compounds by LRMS

Categories identified in the three sample types by LRMS are shown in Appendix G by LC fractions. The LC fraction, the category name, and relative abundances (100, 10, or 1) are given in the table. In many cases, particularly for Laboratories C and D, the TCO and Grav analyses did not "trigger" a LRMS analysis. These fractions are indicated by "NR." In addition, the "trigger" values originally used by Lab C were the Grav values, only, and these were not calculated back to the source. When the values were recalculated, a number of fractions triggered a LRMS analysis. Since the Grav samples had been preserved, it was possible for Lab C to obtain low resolution mass spectra. These results are included in a separate appendix (Appendix H).

TABLE 18. IR RESULTS: ARTIFICIAL SAMPLE IN CH_2CL_2, ALIQUOT 1

Functional Group	Lab A $\bar{\nu}$ cm^{-1}	Lab B $\bar{\nu}$ cm^{-1}	Lab D $\bar{\nu}$ cm^{-1}
OH or NH	3,300(M)	3,600-2,300(W)	---
Aromatic CH or alkyl OH	3,050(M)	3,100-3,000(M)	3,050(W)
Aliphatic CH	2,950, 2,925, 2,850(W)	3,000-2,800(S)	2,960, 2,930, 2,850(S)
Ester (aldehyde; saturated ketone)	1,730(S)	1,720(M)	1,720(M)
Acid C=O	1,700(M)	1,710(M)	---
Aromatic C=C (cyclic C=N)	1,600(S); 1,500(M)	1,600, 1,590, 1,497(M)	1,595, 1,490(M)
$C-NO_2$ (Amide)	1,530(S)	1,530, 1,342(S)	---
CH_3 (Arom C=C)	1,450(M)	>1,370-1,360(M)	---
Ester; ether; alcohol	1,270(S); 1,120(M)	1,270, 1,118(M)	1,265(S); 1,195(W)
Phenol; acid	1,230(M)	---	---
Benzene substitution	1,160(W)	---	1,195(W)
Alcohol; substituted aromatic ring	1,100-1,000(M)	---	---
Substituted aromatic ring	850-700(M)	830-680(M)	815, 775(S)

TABLE 19. IR RESULTS: ARTIFICIAL SAMPLE ON FLYASH MATRIX, ALIQUOT 1

Functional group	Lab A $\bar{\nu}$ cm^{-1}	Lab B $\bar{\nu}$ cm^{-1}	Lab D $\bar{\nu}$ cm^{-1}
OH or NH	---	3,600-2,500(M); 3,500-3,100(M)	3,400(W)
CH, aromatic or olefinic	3,050, 3,020(M)	3,100-3,000(M)	3,080(W); 3,060(M); 3,020(S)
Aliphatic CH	2,960, 2,920, 2,850(S)	3,000-2,800(S)	2,980, 2,950(M) 2,920(S)
Ring vibrations; N-C=N	1,600(M); 1,490(M)	1,590, 1,490(M)	1,600(S), 1,495(S)
C=0; conjugated or amide I	---	1,690-1,660(W)	---
CH_3; CH_2	1,460-1,440(M)	1,460, 1,450(M)	1,455(S)
CH_3	1,370, 1,340(M)	<1,370	---
Aromatic alcohols	---	---	1,375, 1,350(M)
Aliphatics; primary alcohols; aromatics	---	---	1,030(M)
Substituted benzene	750, 690(S)	750, 695(S)	755, 700(S)

TABLE 20. IR RESULTS: FIELD SAMPLE, XAD-2 EXTRACT, RUN 1

Functional group	Lab A ν cm^{-1}	Lab B ν cm^{-1}	Lab D ν cm^{-1}
OH or NH	3,400(W)	3,600-3,300(W)	3,420(W)
Aromatic CH	3,050(M)	3,100-3,000(S)	3,050(S)
Aliphatic CH	2,950, 2,930, 2,850(M)	3,000-2,800(M)	2,960, 2,920 2,850(M)
Combination bands, aromatic	---	2,000-1,650(W)	---
Ketone; α-Cl ketone; esters; aldehydes	1,730(W)	---	1,710(W)
C=0, acidic	---	1,710(M)	---
Ring vibrations; N-C=N	1,600(M); 1,500(W)	1,595, 1,495(M)	1,600(M)
CH_3; CH_2; aromatic CH_3; CH_2Cl	1,460-1,430(M) 1,380(W)	---	1,455, 1,440(M)
Alkanes; amines; esters; alcohols	---	---	1,300(W) 1,300(W)
Esters; ketones	---	---	1,240(W)
Esters; phenols; ether	1,200(W)	---	1,180(W)
Aromatic substitution	840-700(S), multiple	900-700(S)	865-715(M-S) multiple
C-Cl	740(S)	---	---

To evaluate the effectiveness of the LRMS trigger, the LC fractions meeting the weight criterion for LRMS, as well as the LC fractions for which spectra were actually obtained, are tabulated in Table 21. The largest discrepancy noted was in the artificial sample in methylene chloride. Although this sample was judged to be the "simplest," Labs A and B met the weight criterion on seven of the eight fractions, Lab C on five fractions (after recalculating back to the source) and Lab D met the criterion on only one fraction. While fractional overlap could account for some differences in the number of fractions which trigger a LRMS, it would not account for the fact that Lab D triggered on only one fraction. As discussed above, Lab D consistently reported lower gravimetric values than the other labs. Gravimetric values in the range of the other labs would have resulted in a LRMS "trigger" in many cases.

A comparison of categories identified by LRMS in the artificial sample in methylene chloride is given in Table 22. Of a total of thirteen categories identified by one or more labs, only two categories were identified by all four labs. The fraction numbers in parentheses indicate that the laboratory identified the category by IR but not by LRMS. Since Level 1 is "designed to show within broad general limits the presence or absence, the approximate concentrations, and the emission rate of inorganic elements, selected inorganic anions, and classes of organic compounds," these results fall short of the expectations of a Level 1 analysis. Carelessness early in the analysis scheme (LC procedures, TCO and Grav procedures) will result in failure to trigger all the LRMS analyses that should be performed, and organic category information will be lost.

Subcategories and specific compounds by LC fraction are given in Appendix I. The reporting format for Level 1 indicates that these increasingly more specific data should be reported where appropriate and if possible to do so from the spectra. The lack of data from Labs C and D precludes comparison of compounds for each of the samples across the four labs. However, Labs A and B showed a 34% overlap of compounds identified for Sample 1, 21% for Sample 2, and 34% for Sample 3.

Table 23 lists the known components of the artificial sample in methylene chloride (Sample 1) and indicates in which fraction(s) each was identified (if at all) by each of the four laboratories. Although Level 1 is not

TABLE 21. LC FRACTIONS WHICH TRIGGERED LRMS vs. LRMS OBTAINED

Artificial sample in $MeCl_2$	Lab A		Lab B		Lab C		Lab D	
	>0.5 mg/m^3	LRMS	>0.5 mg/m^3	LRMS	>0.5 mg/m^3	LRMS	>0.5 mg/m^3	LRMS
LC1	✓	✓	✓	✓	✓			
LC2	✓	✓		✓	✓			✓
LC3	✓	✓	✓	✓	✓	✓		
LC4	✓	✓	✓	✓	✓	✓		
LC5	✓	✓	✓	✓				
LC6	✓	✓	✓	✓	✓	✓	✓	✓
LC7		✓	✓	✓				
LC8	✓	✓	✓	✓				
Artificial sample on flyash								
LC1	✓	✓	✓	✓				✓
LC2		✓		✓			✓	✓
LC3	✓	✓	✓	✓				✓
LC4		✓		✓				✓
LC5		✓		✓				✓
LC6	✓	✓	✓	✓	✓			
LC7		✓		✓				✓
LC8		✓		✓			✓	✓
XAD-2 extract								
LC1		✓		✓	✓			
LC2	✓	✓		✓			✓	✓
LC3	✓	✓	✓	✓	✓	✓	✓	✓
LC4		✓	✓	✓	✓	✓		
LC5	✓	✓		✓				
LC6	✓	✓	✓	✓	✓	✓	✓	✓
LC7		✓	✓	✓				
LC8		✓	✓	✓			✓	✓

TABLE 22. CATEGORIES IDENTIFIED BY LRMS IN ARTIFICIAL SAMPLE IN CH_2CL_2, ALIQUOT 1

Categories	LC fraction(s) in which category was identified Lab A	Lab B	Lab C	Lab D
Aliphatic hydrocarbons	1,2	1,2	(1)*	2
Halogenated aromatic HC's	2			
Fused alt/non-alt HC's	2,3,4,5	3,4,5	3,4	2
Heterocyclic S compounds	2,3,4			
Esters, phthalates	4,5,6,8	(6,7)	4,6	2
Aromatic HC's, benzenes	3,4,5	3	3,6	(2,4,5,6)
Nitro aromatic HC's	(4,5)	4,5,6	(4,5,6)	
Heterocyclic N	4,6,7,8			
Carboxylic acids, derivatives	5,6,7,8	4,5,6,7	6	6
Ethers	6,7,8			(2)
Phenols	6,7,8	6		(4,5)
Sulfonic acids, sulfoxides	6,7		(6)	6
Inorganics	8			

*Fraction numbers in parentheses indicate that the category was identified by IR but not by LRMS.

TABLE 23. SPECIFIC COMPOUNDS IDENTIFIED BY LRMS IN ARTIFICIAL SAMPLE IN METHYLENE CHLORIDE, ALIQUOT 1

Composition	LC fraction(s) in which category was identified			
	Lab A	Lab B	Lab C	Lab D
Squalane	1,2	1,2		
n-Tridecane				
Biphenyl	2,3	3		
Chlorobenzene	2			
Acenaphthene	2,3	3		
Chrysene	2,3,4,5	3,4,5	3,4	2
Dihexylether	(7,8)*			
Dinitrotolurene	4,5	4,5,6		
Dibenzothiophene	2,3,4	(3,4)		(2)
Diethylphthalate	4,6	6		
2-Ethylhexanol				
Phenol	6	6		
Quinoline	6,7,8			
Palmitic acid	6,7,8	6,7		
Stearic acid	6	6,7		
Di-p-tolylsulfoxide	6,7	(6,7,8)		

*Fraction numbers in parentheses indicate peaks at the appropriate m/e which were either unidentified or identified as another compound.

designed to identify specific compounds, the results are disappointing in that Labs C and D each identified only one of the sixteen components.

Categories identified by LRMS in the artificial sample on a flyash matrix are given in Table 24. Lab C reported no low resolution mass spectra for this sample. Of a total of seventeen categories identified by one or more of the remaining labs, only five were identified by all three. These results are also outside the limits of a Level 1 analysis.

Table 25 lists the components of the artificial sample on a flyash matrix and indicates in which fraction(s) each was identified (if at all) by each of the four laboratories. The large number of peaks that were either unidentified or identified as another compound (indicated by the fraction numbers in parentheses) points to a possible problem with the interpretation of the low resolution mass spectra.

INORGANIC ANALYSIS RESULTS

The Phase-II flyash sample aliquots were Parr-bombed in accordance with Level 1 procedures and sent to independent laboratories for analysis by spark source mass spectrometry (SSMS), with the exception of the sample from Laboratory D which was sent directly to the SSMS analyst with no pretreatment. Results are given in Table 28. In most of the cases shown, the high and low values for a given element differ by a factor greater than 3. Nickel and beryllium, which have the lowest MATE values of the elements shown, were found to range from 13 to 380 ppm and from 0.5 to 14 μg/g, respectively.

The SSMS analyses for Contractors C and D were performed by the same outside laboratory. However, since Contractor C's sample was Parr-bombed and Contractor D's was not, this cannot be considered a true intralaboratory test of the SSMS technique.

Included in the table are values for arsenic and antimony, two of the elements for which alternate procedures were specified in Level 1. A comparison of these SSMS values to the values obtained by the recommended silver diethyldithiocarbamate (SDDC) method for arsenic and the atomic absorption method for antimony is given in Table 29. For Sb, the values obtained by AA are slightly less than those by SSMS in both cases. For arsenic, however, the differences are much greater with the SDDC value being higher than the SSMS value in one case and lower in the other.

TABLE 24. CATEGORIES IDENTIFIED BY LRMS IN ARTIFICIAL SAMPLE ON FLYASH MATRIX, ALIQUOT 1

	LC fraction(s) in which category was identified			
	Lab A	Lab B	Lab C	Lab D
Aliphatic hydrocarbons	1			1
Halogenated aliphatics		1	no LRMS reported	
Aromatic HC's				
benzene, substituted benzenes	2,3,4,5	3,4		1,2,3,4
Halogenated aromatic HC's	1,6	1,2		1
Fused alternate, non-alternate HC's	3	3,4,5,6,7		2
Heterocyclic N compounds	3,4,5,6,7,8	3,4,5,6,7,8		3,4,5
Ketones	4			
Heterocyclic O compounds				4
Heterocylic S compounds	4,5			4,6
Esters	4,5,7,8			
Phenols	5,6,7,8	6,7		5
Amines	6,7			5,6
Carboxylic acids and derivatives		5,6,7,8		5,6,8
Alcohols				6,7
Amides	6,7			6
Sulfur	1,3,4			
Inorganics	8			

TABLE 25. SPECIFIC COMPOUNDS IDENTIFIED BY LRMS IN ARTIFICIAL SAMPLE ON FLYASH MATRIX, ALIQUOT 1

	LC fraction(s) in which category was identified			
	Lab A	Lab B	Lab C	Lab D
Styrene	3,4,5	(7,8)*	no LRMS reported	
Biphenyl/acenaphthene				
Diphenylmethane				
Anthracene/phenanthrene	3,4	3,4,5,6,7		2
Stilbene/methylenefluorene	3,4,5	3,4		2
Diphenylethane		(3,4,5,6,7,8)		
Methylenephenanthrene				
Methylphenanthrene	3	(3,4)		(2)
Diphenylpropene/methylstilbene	3,4,5	(3,4)		
Diphenylpropane				
Phenylnaphthalene	(4)	(3,4)		
Dimethylphenanthrene		(3,4)		(2)
Methylphenylindan/ hexahydropyrene	(3,4,5)	(3,4)		(2)
Diphenylbutane	4	(3,4)		
Diphenylthiophene	5	(3)		(2)
Methylchrysene	(4,5)			
α-Methylstyrene	3,6			
Cumene				
Cumyl alcohol	(4,5)			
Acetophenone				
Hexachlorobutadiene		1		
Hexachlorobenzene	1	1		2
Hexachloroethane	(5)	(3)		
Pentachlorobenzene				
Phenol	6	6		5
Cresol	6	6		
Quinoline	3,5,6,8	4,5,6,8		3,5
Aniline	6,7			
Indole	4,5	4,5		3
Benzoic acid				

*Fraction numbers in parentheses indicate peaks at the appropriate m/e which were either unidentified or identified as another compound.

TABLE 28. SSMS RESULTS:* ARTIFICIAL SAMPLE ON FLYASH MATRIX (μg/g)

Element	Lab A	Lab B	Lab C	Lab D
Uranium	2.2	2.5	3	90
Thorium	4.7	5.1	8	75
Bismuth	0.48	1.8		0.4
Lead	15	33	8	24
Thallium	<2.0	0.95	0.3	0.3
Mercury		NR	NR	
Gold		0.25	≤0.2	<0.2
Platinum		7.2	2	<0.2
Iridium		1.1		<0.2
Osmium				<0.2
Rhenium		STD		≤0.3
Tungsten	<2.1	5.8	3	6
Tantalum		1.6	≤0.4	≤2
Hafnium		17	0.5	3
Lutetium		0.66	0.2	0.6
Ytterbium	<1.9	2.2	2	8
Thulium		1.1	0.3	0.5
Erbium	<2.2	5.0	0.9	12
Holmium	0.36	0.91	1	16
Dysprosium		9.4	2	25
Terbium		4.4	0.4	6
Gadolinium	3.1	16	2	15
Europium	0.62	3.5	0.7	8
Samarium	<3.6	2.5	4	27
Neodymium	9.3	12	5	36
Praseodymium	1.4	5.4	2	27
Cerium	1.4	23	12	170
Lanthanum	11	18	19	180
Barium	210	~0.5%	MC	
Cesium	0.43	1.0	0.7	2
Iodine	<0.19	0.54	<0.1	2
Tellurium	<0.53	0.25	≤0.2	≤1
Antimony	2.4	6.9	1	0.8
Tin	3.1	11	2	5
Indium		STD	STD	STD
Cadmium	4.1	14	3	0.4
Silver		0.90	≤0.4	1
Palladium	<1.0			<0.2
Rhodium	<0.19			<0.2
Ruthenium				<0.2
Molybdenum	1.3	8.7	7	15
Niobium	3.3	56	160	30
Zirconium	52	300	99	
Yttrium	35	41	38	
Strontium	MC	≈3,100	MC	

(continued)

TABLE 28 (continued)

Element	Lab A	Lab B	Lab C	Lab D
Rubidium	8.6	7.5	4	11
Bromine	150	9.6	2	5
Selenium	6.5	41	5	13
Arsenic	59	41	38	140
Germanium	2.9	6.0	2	12
Gallium	6.3	4.9	15	42
Zinc	31	21	67	20
Copper	41	42	41	120
Nickel	25	59	380	13
Cobalt	9.1	2.7	23	10
Iron	MC	>1%	MC	
Manganese	230	200	470	
Chromium	6.9	66	160	100
Vanadium	39	58	26	130
Titanium	600	≈1,700	MC	
Scandium		4.0	9	50
Calcium	MC	>1%	MC	
Potassium	930	≈3,200	MC	
Chlorine	520	210	58	290
Sulfur	MC	2,400	MC	
Phosphorus	420	800	MC	
Silicon	MC	>1%	MC	
Aluminum	MC	>1%	MC	
Magnesium	MC	>1%	MC	
Sodium	MC	>1%	MC	
Fluorine	210	450	MC	230
Oxygen		NR	NR	
Nitrogen		NR	NR	
Carbon		NR	NR	
Boron	2.2	200	4	
Beryllium	1.1	0.60	0.5	14
Lithium		32	>130	>360
Hydrogen			NR	

*Results are reported as received from the laboratories;
STD = internal standard.

Lab A: MC = major component; elements for which values are not entered were not reported.

Lab B: All elements for which values are not entered <0.1 ppm weight; NR = not reported.

Lab C: NR = not reported; all elements not reported <0.1 ppm weight.

Lab D: All elements for which values are not entered were not reported.

TABLE 29. COMPARISON OF As AND Sb BY SSMS AND BY SDDC AND AA, RESPECTIVELY

	As, µg/g		Sb, µg/g	
	SDDC	SSMS	AA	SSMS
Lab A	100	59	0.04	2.4
Lab B				
Lab C	775	38	<1	1
Lab D	35	140	<0.05	0.8

In a separate test of the spark source mass spectrometric technique, RTI sent four audit samples to an outside laboratory for analysis by SSMS. Two of the samples (Aliquots 1 and 2) were identical and were prepared in a low organics matrix (Treatment 1); the other two samples, also identical, were in a high organics matrix (Aliquots 1 and 2 for Treatment 2). Each of the samples was weighed and ashed using a low temperature asher. It should be noted that the sample preparation used for this experiment is not the recommended Level 1 procedure.

The analysis results, as reported by the outside laboratory, are presented in Table 30 for twelve elements. For each element, treatment, and aliquot, the mean of three replicate analyses and the standard deviation about the mean are given along with the known (RTI) value (determined gravimetrically during sample preparation) for selected elements.

To summarize the data in Table 30, it is seen that:

a. The treatment effect was significant at the 0.10 or greater level for 10 of the 12 elements. In general, the low organic (Treatment 1) sample resulted in lower values than the high organic (Treatment 2) sample.

b. The aliquot effect within treatments was not significant at the 0.10 level for 11 of the 12 elements.

c. Testing the mean values from 12 analyses per element from the outside laboratory with the RTI value showed the difference to be not significant at the 0.10 level for 11 of 12 elements.

d. Testing the mean value from 6 analyses of Treatment 1 samples against the RTI value showed the difference to be not significant at the 0.10 level for 10 of the 12 elements.

TABLE 30. RESULTS OF TESTS OF SIGNIFICANCE* AND SAMPLE STATISTICS BY ELEMENT

	Outside laboratory								
	Significance tests		Mean values(µg/g) (std. deviation, µg/g)				Significance test outside lab vs. RTI (combined treatments‡)		Significance test, outside lab, vs. RTI (treatment 1 only§)
	Treatment effect	Aliquot(T) effect							
Element	T	A	T1 A1†	T1 A2	T2 A1	T2 A2		RTI(µg/g)	
V	Sig(.05)	N.S	107 (67)	88 (24)	166 (28)	156 (46)	N.S.	107	N.S.
Cr	Sig(.05)	Sig(.05)	425 (104)	254 (77)	299 (73)	172 (27)	Sig(.10)	66	Sig(.10)
Mn	N.S.	N.S.	252 (105)	145 (25)	221 (61)	269 (114)	N.S.	247	N.S.
Ni	Sig(.10)	N.S.	52 (24)	41 (2)	71 (9)	71 (38)	N.S.	49	N.S.
Cu	Sig(.10)	N.S.	66 (37)	63 (1)	96 (32)	134 (60)	N.S.	64	N.S.
Zn	Sig(.10)	N.S.	98 (59)	101 (9)	193 (93)	145 (29)	N.S.	145	N.S.
As	Sig(.05)	N.S.	15 (3)	20 (3)	33 (9)	37 (16)	N.S.	31	Sig.(.05)
Se	Sig(.10)	N.S.	10 (6)	11 (3)	19 (2)	13 (4)	N.S.	5	N.S.
Cd	N.S.	N.S.	14 (9)	11 (3)	21 (24)	7 (4)	N.S.	.7	N.S.
Pb	Sig(.01)	N.S.	39 (3)	47 (6)	73 (8)	57 (15)	N.S.	35	N.S.
Th	Sig(.10)	N.S.	6 (3)	10 (0)	5 (5)	3 (2)	N.S.	12	N.S.

See footnotes at end of table.

(continued)

TABLE 30 (con.)

	Outside laboratory								
	Significance tests								
	Treatment effect	Aliquot(T) effect	Mean values(µg/g) (std. deviation, µg/g)				Significance test outside lab vs. RTI (combined treatments‡)		Significance test, outisde lab, vs. RTI
Element	T	A	T1 A1†	T1 A2	T2 A1	T2 A2		RTI(µg/g)	(treatment 1 only§)
U	Sig(.10)	N.S.	6 (3)	10 (0)	6 (4)	3 (2)	N.S.	6	N.S.

*Sig.(.10) = significant at 0.10 level,
Sig.(.05) = significant at 0.05 level,
Sig.(.01) = significant at 0.01 level,
N.S. = not significant.

†T1 A1 = treatment 1, aliquot 1, etc.

‡Combined treatments 1 and 2; tested RTI's one value versus mean of 12 outside laboratory values (i.e., overtreatment and aliquot).

§Treatment 1 only; tested RTI's one value versus mean of 6 outisde laboratory values (i.e., over aliquots for treatment 1 only).

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2. "Method 1--Sample and Velocity Traverses for Stationary Sources," Federal Register, Volume 42, No. 160 (Thursday, August 18, 1977) p. 41755.

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APPENDIX A

COMPOSITION OF
PHASE II
ARTIFICIAL SAMPLES

TABLE A-1. ARTIFICIAL SAMPLES IN METHYLENE CHLORIDE

	Composition - mg/20 mls		
	Sample Nos. 1-6 (79347-161)	Sample Nos. 7-12 (79734-162)	Sample Nos. 13-18 (79347-163)
Squalane	12.7	12.7	7.6
n-Tridecane	14.4	8.6	14.4
Biphenyl	13.6	13.6	13.6
Chlorobenzene	20.1	12.1	40.2
Acenaphthene	14.0	14.0	8.4
Chrysene	15.7	9.4	15.7
Dihexylether	17.8	17.8	17.8
Dinitrotoluene	20.1	12.1	40.2
*Dibenzothiophene	12.7	12.7	7.6
Diethylphthalate	14.4	8.6	14.4
2-Ethylhexanol	15.4	15.4	15.4
Phenol	16.7	10.0	33.4
Quinoline	12.6	12.6	7.6
Palmitic acid	13.3	8.0	13.3
Stearic acid	12.2	12.2	12.2
**Di-p-tolylsulfoxide	20.4	12.2	40.8
Total	246.1	192.0	302.6

* Dibenzofuran was not available in stock.

** p-Toluene sulfonic acid has insufficient solubility for preparation of these samples.

TABLE A-2. ARTIFICIAL SAMPLES ON FLYASH MATRIX

Samples Nos. 19-35

Each sample contains about 5 g of flyash dosed at a level (per 5 g) of:

50 mg Styrene waste	-	mixture of aromatic hydrocarbons
53 mg API waste extract		mixture of aliphatic unsaturated hydrocarbons and aromatic hydrocarbons
50 mg Lucidol waste	-	mixture of α-methylstyrene, cumene, cumyl alcohol, and acetophenone
50 mg Perchloroethylene waste	-	hexachlorobutadiene, hexachlorobenzene, and a mixture of other chlorinated hydrocarbons
56 mg Simulated coke waste extract	-	mixture of phenol, cresol, amines and benzoic acid
25 mg p-Toluene sulfonic acid		

More detailed descriptions of the wastes are attached.

(continued)

TABLE A-2. (continued)

Styrene waste extract composition	- 98.6% soluble
Styrene	1.8%
Biphenyl/acenapthene	6.0%
Diphenylmethane	5.5%
Anthracene/phenanthrene	21.8%
Stilbene/methylfluorene	15.5%
Diphenylethane	10.4%
Methylenephenanthrene	2.5%
Methylphenanthrene	1.8%
Diphenylpropene/methylstilbene	7.6%
Diphenylpropane	7.3%
Phenylnapthalene	3.5%
Dimethylphenanthrene	1.1%
Methylphenylindan/hexahydropyrene	1.8%
Diphenylbutane	2.9%
Diphenylthiophene	1.1%
Methyl chrysene	1.6%
	92.2%

(continued)

TABLE A-2. (continued)

API waste extract composition		-	13% soluble
Aliphatics		42.7%	
2n + 3	7.7%		
2n	9.3		
2n - 2	6.5		
2n - 4	4.1		
2n - 6	6.3		
2n - 8	4.8		
2n - 10	4.0		
Aromatics	MW <178	14.1%	
Aromatics	MW >178 <216	24%	
Aromatics	MW >216	6.3%	
		87%	

(continued)

TABLE A-2. (continued)

Cumene peroxide waste = "lucidol waste"

40%	α-Methylstyrene
32%	Cumene
18%	Cumyl alcohol
3%	Acetophenone
0.3%	Water

Perchloroethylene waste composition

Hexachlorobutadiene	65%
Hexachlorobenzene	6.5%
Hexachloroethane	1%
Pentachlorobenzene	2.5%

Others at 1-5%; all chlorinated

(continued)

TABLE A-2. (continued)

Simulated coke plant waste

Component	mg Taken for simulated waste	% Abundance in real waste
Phenol	640	60
o-Cresol	253	27
Quinoline	91	5
Aniline	72	4
Indole	55	5
Benzoic acid	10	≤ 1

APPENDIX B

PHASE I INFRARED SPECTROSCOPY RESULTS: FUNCTIONAL GROUPS IDENTIFIED IN LIQUID CHROMATOGRAPHY FRACTIONS

TABLE B-1. FUNCTIONAL GROUPS IN CYCLONE EXTRACT LC FRACTION IDENTIFIED BY IR

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
1	3,400	W	OH, NH	3,400	W(broad)	OH, NH
	2,950, 2,920	S	Aliphatic C-H	2,920	S	Aliphatic C-H
	2,850	M	CH_2			
	1,460	M	CH_2, CH_3	1,460	M	CH_2
	1,380	M	CH_3	1,375	M	CH_3
				1,050	W(broad)	C-OH
2	3,400	M	OH, NH	3,400	W(broad)	OH, NH
	2,950, 2,920	S	Aliphatic C-H	2,920	W	Aliphatic C-H
	2,850	M	CH_2			
	1,450	W	CH_2, CH_3			
	1,380	M	CH_3	1,000	S	Silica gel
3	3,050	M	Aromatic C-H	3,050	M	Unsaturated CH
	2,920	W	Aliphatic C-H	2,920	VW	Saturated CH
				1,930	W	Allene
	1,600	M	Ring vibrations	1,600	M	Aromatic ring
	1,460-1,440	M	Aromatic C-H	1,450	M	CH_2
	1,260	M	CH_2CL, nitroso dimer, C-O-NO_2, S-CH_2, $SiCH_3$			
	900-700	S	Substituted aromatic, fused rings	850-700	S (multiplets)	Aromatic fused rings, substituted pyridine

(continued)

TABLE B-1 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
4	3,400	M	OH, NH	3,400	M(broad)	OH, NH
	3,050	M	Aromatic C-H	3,050	M	Unsaturated CH
	2,920	W	Aliphatic C-H	2,920	W	Saturated CH
				1,700	M	Ketone, ester, carbamate, imide
	1,600	M	Ring vibrations	1,600	M	Aromatic ring N-NO_2
	1,450	M	Aromatic C-H, $SiCH_2$	1,450	M	CH_2, CH_3
	1,380	M	CH_3, $SiCH=CH_2$			
	1,200	M(broad)	$SiCH_2$, phenol, $H_2C = CHOCH_2$			
				1,050	M(broad)	Ester, ether, alcohol
	750	S	Aromatic, fused ring	810-750	M-S (multiplets)	Substituted aromatic, fused rings, substituted pyridine
5	3,400	W	OH, NH	3,400	M(broad)	NH, OH
	3,050	W	Aromatic C-H	3,050	M	Unsaturated CH
	2,920	W	Aliphatic C-H	2,920	M	Saturated CH
	2,220	W	C≡N	2,220	W	C≡N
				1,930	W	Allene
	1,700	S	Cyclic imide, imide, carbamate, aromatic aldehyde, conjugated ketone, unsubstituted amidine, HCL	1,700	S(sharp)	Imide, carbamate, lactam, ester, ketone

(continued)

TABLE B-1 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
5	1,600	M	Ring vibrations	1,600	M	Aromatic ring
	1,450	M	Aromatic CH_2, CH_2	1,450	M	CH_2, CH_3
				1,200-1,000	M(very broad)	C-O, ester, ether, alcohol
	820	W	Substituted pyridine	820	M	Substituted aromatic substituted pyridine
	750	S	Substituted aromatic, fused rings	750	S	Substituted aromatic, substituted pyridine, fused rings
6	3,400	W	OH, NH			
				3,300	M(broad)	NH, OH, NH_4^+, C≡CH
	3,050	M	Aromatic C-H	3,050	M	Unsaturated CH
	2,950, 2920	M	Aliphatic C-H	2,920	M	Saturated CH
	2,850	M	CH_2			
				2,220	W	C≡N
				1,930	W	Allene
	1,720	S	Imide, carbamate, lactone (6-membered), lactam (5-membered), ketone			
				1,700	S	Ketone, imide, carbamate, lactam ester
				1,650	S	Amide, ketone $O-NO_2$ O-N=O, C=N
	1,620-1,600	S	C=C, ring vibrations	1,600	S	Aromatic ring $N-NO_2$
	1,450	M	Aromatic C-H, aliphatic C-H	1,450	S	CH_2, CH_3

(continued)

TABLE B-1 (continued)

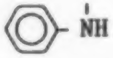
	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
6	1,300-1,200	M(broad)	C-O, ester, ether	1,250	S	Ester, ether, phenol, alcohol
	750	S	Substituted aromatic, fused rings	810 750	M S	Substituted aromatic substituted pyridine, fused ring compounds
7	3,400	S(broad)	OH, NH	3,400	S(broad)	NH, OH
	3,050-3,020	M	Aromatic C-H			
	2,950	M	Aliphatic C-H	2,920	W	Saturated CH
	1,730	M	Imide, carbamate, lactone, lactam, ketone			
	1,630	M	C=C, $-CH_2O-NO$	1,620	M	C=C, $SiCH=CH_2$
	1,600	M	Ring vibrations, CH_2ONO			
	1,450	M	CH_2, CH_3			
	1,380	S	$SiCH=SiCH_3$	1,380	S(sharp)	$SiCH=CH_2$ inorganic salt
	1,280	M	CH_2-CL, $SiCH_3$			
	750	M	Aromatic, fused rings			
8	3,400	S(broad)	OH, NH			
	2,220	W(broad)	C≡N			
	1,620	S	Substituted olefin			
	1,400	W	Substituted olefin			
	1,150	M	Possibly tertiary alcohol			
	600	S	Substituted olefin			

TABLE B-2. FUNCTIONAL GROUPS IN XAD-2 EXTRACT LC FRACTION IDENTIFIED BY IR

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
1	3,450	VW(broad)	NH_4, OH			
	2,950, 2,930	M	Aliphatic CH	2,950, 2,920	S	Aliphatic C-H
				2,850	S	Aliphatic C-H
	1,470	W	Aliphatic CH			
				1,450, 1,375	W	Aliphatic C-H
	1,390	W	Possibly NH_4 salt			
2	3,400	VW(broad)	NH, OH			
				3,050	W	Aromatic C-H
	3,040	M	Aromatic CH			
	2,930	M	Aliphatic CH	2,950, 2,920	M	Aliphatic C-H
				2,850	M	Aliphatic C-H
				1,730	W	Ester
	1,600, 1,500	M	Ring vibrations			
	1,450-1,430	M	Aliphatic CH			
	1,380-1,360	M	Aliphatic CH			
	1,240		Aliphatic CH, possibly Si			
				1,100-1,000	W	Possibly silica, possibly alcohol
	830-700	S	Substituted benzene, fused ring compounds	900-700	W	Substituted aromatic
3				3,400	W(broad)	OH, NH
	3,050	M	Aromatic CH	3,050	M	Aromatic C-H
	2,930	W	Aliphatic CH			
				2,920	W	Aliphatic C-H
	1,600, 1,500	W	Ring vibrations			
	1,450-1,430	M	Aliphatic CH			
	830-700	S	Substituted benzene, fused rings	700-900	S	Substituted aromatic, fused rings

(continued)

TABLE B-2 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
4				3,410	M	NH
	3,400	S	NH	3,600-3,200	W(broad)	NH, OH
	3,050	M	Aromatic CH	3,050	M	Aromatic C-H
	2,950-2,920	W	Aliphatic CH	2,950-2,850	W	Aliphatic C-H
	1,640	M	C=C			
	1,600, 1,500	M	Ring vibrations			
	1,450	S				
	1,330, 1,320	M	 NH			
	1,240	M				
	800-700	S	Substituted aromatic ring	900-700	S	Substituted aromatic, fused rings, possibly dibenzothiophene
5	3,400	M(broad)	OH, NH	3,400	S(broad)	OH, NH
	3,050	M	Aromatic C-H	3,050	M	Aromatic C-H
	2,950-2,930	M	Aliphatic C-H	2,950-2,850	S	Aliphatic C-H
				2,230	M	C≡N or C≡C
	2,220	M	C≡N			
	1,700	S	C=O (ester)	1,700	S	Ketone, carboxyl
	1,620	M	C=C			
	1,600, 1,580	M	Ring vibrations	1,600	S	Conjugated C=C, aromatic C=C, cyclic C=N, N-NO_2, C-N=O, carboxylate ion
				1,530	M	C=N, C-$\underset{+}{N}O_2$
	1,440	M	Aliphatic C-H	1,450, 1,420	S	CH_3, NH_4^+
				1,300-1,050	M	Multiple peaks, alcohol, phenol, ester, amines, C-CL, C=S, Si-O-Si, C-F

(continued)

TABLE B-2 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
5	1,200-1,000	M(broad)	C-O (ester)			
	750	S	Aromatic ring	850-700	S	Substituted aromatics
6	3,400-3,300	M(broad)	OH, NH	3,300	M(broad)	OH, NH
	3,050	M	Aromatic C-H	3,050	W	Aromatic C-H
	2,950-2,930	M	Aliphatic C-H	2,950-2,850	M	Aliphatic C-H
	1,780, 1,720	S	C=O (ketone)	1,780	W	Anhydrides, peroxide, ester, lactones
				1,720	S	Ketone, ester
	1,600	M	Ring vibrations	1,600	S	C=C, C=N, N-NO_2, C-N=O, CO_2
				1,530	M	C=N, C-NO_2
	1,450	M	Aromatic and aliphatic, C-H	1,450, 1,420	S	CH_3, NH_4^+
	1,380	M	Possibly $CH_3\overset{O}{\overset{\|}{C}}$-			
	1,300-1,200	M	ϕ-$\overset{\|}{C}$	1,270, 1,230	S	Ester, alcohol, amine, amide, SO_3R, P=O
				1,100	S(broad)	Alcohol, ether, phosphate, silicate
	750, 710	M	Aromatic ring	750, 720	S	Substituted aromatics
7	3,400	S(broad)	H_2O, OH	3,400	S(broad)	OH, NH
	2,950-2,930	M	Aliphatic C-H	2,950-2,850	W	Aliphatic C-H
				1,730, 1,710	M	Ester, ketone, acid
	1,630	S	C=C, amide	1,630	M	C=C, N-C=N, C=N, $SiCH=CH_2$
	1,600	S	Aromatic ring			
	1,550	S	Amide, CH_2-NO_2			
				1,450	M	CH_2, CH_3

TABLE B-2 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
7	1,420	S	Aliphatic C-H			
	1,380	S(Sh)	$SiCH=CH_2$, inorganic Salt, CH_2-NO_2	1,380	M	CH_3, $\underset{\diagup O}{\overset{\diagdown}{N}}=\underset{\diagdown O}{\overset{\diagup}{N}}$, $SiCH-CH_2$
				1,250, 1,220	S	CH_2CL, CH_2BR, CH_2S, phenol, α, ∞, unsaturated ester
				1,100	W	2° alcohol, SO_4
	1,060	M	C-O (alcohol)			
				1,000, 980	M	$SiCH=CH_2$, SiC_2H_5, $CH_2=$ CH-
				810	M	Melamine, $CH_2-O-CH=CH_2$, $R_2C=CHR$
8	3,200	S(broad)	NH_4			
	1,400	S	NH_4 salt			

TABLE B-3. FUNCTIONAL GROUPS IN SORBENT MODULE RINSE LC FRACTION IDENTIFIED BY IR

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
1	3,400	S(broad)	OH	3,400	M-S(broad)	OH, NH
	2,950, 2,920	S	Aliphatic C-H	2,920	S	Saturated C-H
	2,850		Unassigned			
				1,620	W	C=C, O-NO_2, C-N=O, amine salt
				1,450	M	CH_2, CH_3
				1,380	M	CH_3, H_2C=CSi
	1,100-1,000	S	Si-O-Si (silica gel)	1,100-1,000	S(broad)	Si-CH_3, SiOSi
				700	VW	CH_2-NH-CH_2
2	3,400	W(broad)	OH	3,400	S(broad)	OH, NH
	2,950, 2,850	W	Aliphatic C-H	2,920	M	Saturated C-H
				1,640	M	Ketone, C=C, C-NO
				1,380	M	CH_3
	1,100-1,000	S	Si-O-Si (silica gel)			
				650	M(broad)	C=C, C-CL
3	3,400	W	OH, NH			
	3,050	M	Aromatic C-H, C=C	3,050	S	Unsaturated CH
	2,950, 2,850	M	Aliphatic C-H	2,920	M	Saturated CH
	1,930	W	Allene			
	1,730	M	Ester, αCL ketone, lactam, olefin, diketone, aromatic olefin, C=N, N=N, N-NC_2, C-N=O			

(continued)

TABLE B-3 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
3				1,620	M	C=C, N-C=N
				1,600, 1,500	M	Aromatic ring
				1,500-1,400	S (multiplets)	S-CH=CH_2, CH_3, CH_2, S-CH_2, S-CH_3, P-CH_2, Si - ⊙, substituted pyridine
	1,460-1,420	M(multiplets)	CH_3, N-N=O, NH_4^+, aromatic C=C			
	1,380, 1,310, 1,300	W	Sharp peaks			
	1,240, 1180, 1,130	W	Sharp peaks			
	1,170, 1030	W	Ester, alcohol, ether			
	900-700	S	Ring substitution, C-Cl			
				850-700	S (multiplets)	Substituted aromatic, fused rings, substituted pyridine
				620	M	Fused rings, sulfur compounds, Si compounds
4				3,450	W	OH, NH
	3,050	M	Aromatic C-H	3,050	M	Aromatic C-H
	2,920	W	Aliphatic C-H	2,930	W	Aliphatic C-H
	1,930	W	Allene, substituted aromatic			

(continued)

TABLE B-3 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
4	1,600	M	Ring vibrations, C=C	1,600, 1,500	M	Aromatic ring
	1,480-1,420	M(SH)	CH_2, $S-CH_3$, N-N=O, aromatic C=C, C=C	1,470-1,420	M (multiplets)	$S-CH=CH_2$, CH_3, CH_2, $S-CH_2$, $S-CH_3$, $P-CH_2$ Si- ◎, substituted pyridine
	1,260-1,130	M (multiplets)	Carbon skeleton			
	1,100	M(broad)	C-O, ether, C-N-C			
	850-700	S(multiplets)	Aromatic, fused rings	860-700	S	Substituted aromatic rings, fused aromatic rings, substituted pyridine
	615	M	Biphenyls, naphthalene, ether			
5	3,400	W	OH, NH	3,400	W	OH, NH
				3,050	M	Aromatic and unsaturated CH
	3,040	M	Aromatic C-H			
	2,920	W	Aliphatic C-H	2,920	W	Saturated C-H
				2,200	W	C≡N
	1,930	W	Allene, substituted aromatics			
				1,700	M	Ketone, carbamate, imide
	1,600	M	Ring vibrations, C=C	1,600, 1,500	M	Aromatic ring
	1,480-1,420	M(SH)	CH_2, $S-CH_3$, N-N=O, aromatic C=C, C=C	1,450, 1,420	M	CH_2, nitrosamine, CH_3

(continued)

TABLE B-3 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
5	1,260-1,120	M(SH, multiplets)	Carbon skeleton			
	840-700	S(multiplets)	Aromatic, fused rings	850-700	S(multiplets)	Substituted aromatics, fused ring compounds
	615	M	Biphenyls, naphthalenes			
6	3,400	M(broad)	NH, OH	3,400	S(broad)	NH, OH
	3,050	M	Aromatic C-H	3,050	M	Unsaturated C-H
	2,950-2,920	M	Aliphatic C-H	2,920	M	Saturated C-H
				1,770	W	Lactone, imide, ester
	1,710	S	C=O, αCL ketone, dialkyl-ketone, conjugated ester, esters, lactone, lactam, carbamate, imide	1,710	S	Imide, ketone, ester
				1,670	M	Ketone, lactam, C=C
	1,600	S	Ring vibrations, C=C	1,600	S	Aromatic ring, C-N=O $N-NO_2$, boron compound
	1,450	M	CH_3, CH_2, CH_2BR			
				1,440	M	CH_2, CH_3
				1,400-1,200	M(broad)	Ether, ester, acid, alcohol, boron compound

(continued)

TABLE B-3 (continued)

	SASS 1			SASS 2		
LC	$\bar{\nu}$, cm^{-1}	Intensity	Assignment	$\bar{\nu}$, cm^{-1}	Intensity	Assignment
	1,230	S(broad)	C-O, conjugated ester, CH_2-BR, nitroso dimer, S-CH_2			
	1,080	S(broad)	C-O, conjugated ester, alcohol, ether, C-N-C			
				750	S	Substituted aromatic, C-CL, substituted pyridine
	740	S	Cyclic C-CL, NH, substituted aromatic, substituted pyridine			
7	3,400	S(broad)	OH, NH	3,400	S(broad)	OH, NH
				1,700	W	Ketone, imide, $C(NH_2)_2^+$ CL-, carbamate
	1,625, 1,600	S, S	Unsubstituted amide	1,620	S	Amide, C=C
				1,600	S	Amide, amine salt, C-N=O, SiCH=CH_2
	1,400	W(broad)	C-N	1,400	M	C=C, SiCH=CH_2
				1,080	M(sharp)	Unassigned
8				3,400	S	NH
				1,600	S	NH_4-CL
				1,380	S	NH_4-CL

APPENDIX C
CATEGORIES IDENTIFIED IN PHASE I ORGANIC EXTRACTS BY LRMS

TABLE C. CATEGORIES IDENTIFIED IN ORGANIC EXTRACTS BY LRMS

a. Cyclone Extracts	SASS 1			SASS 2		
	Intensity	Category	MW Range	Intensity	Category	MW Range
LC 3	100	Fused alt/non-alt hydrocarbons	128-550	100	Fused alt/non-alt hydrocarbons	128-500
	10	Heterocyclic sulfur compounds	184-234			
LC 6	100	Heterocyclic nitrogen compounds	179-320	100	Heterocyclic nitrogen compounds	129>300
	100	Esters	390			
	1	Carboxylic acids	122	1	Carboxylic acids	122
	1	Phenols	94-108			

b. XAD-2 Extracts	SASS 1			SASS 2		
	Intensity	Category	MW Range	Intensity	Category	MW Range
LC 1	NR			100	Sulfur	256
				10	Aliphatic hydrocarbons	to 400
LC 2	100	Fused alt/nonhydrocarbons	<216	100	Fused alt/nonhydrocarbons	<216
	100	Fused alt/non-alt hydrocarbons	>216	100	Fused alt/nonhydrocarbons	>216
	10	Aromatic hydrocarbons		10	Aromatic hydrocarbons	92-120
	1	Heterocyclic sulfur compounds		10	Heterocyclic sulfur compounds	184-198

(continued)

TABLE C (continued)

b. XAD-2 Extracts (con.)

	SASS 1			SASS 2		
	Intensity	Category	MW Range	Intensity	Category	MW Range
LC 3	100	Fused alt/non-alt hydrocarbons	<216	100	Fused alt/non-alt hydrocarbons	<216
	100	Fused alt/non-alt hydrocarbons	>216	100	Fused alt/non-alt hydrocarbons	>216
	10	Aromatic hydrocarbons	92-168			
	10	Heterocyclic sulfur compounds	184, 234	10	Heterocyclic sulfur compounds	184, 234
LC 4	100	Heterocyclic nitrogen compounds	167-267	100	Heterocyclic nitrogen compounds	167-217
	100	Fused alt/non-alt hydrocarbons	<216	100	Fused alt/non-alt hydrocarbons	<216
	10	Fused alt/non-alt hydrocarbons	>216	100	Fused alt/non-alt hydrocarbons	>216
				10	Heterocyclic sulfur compounds	234
LC 6	100	Unidentified	200-304			
	100	Heterocyclic nitrogen compounds	179	100	Heterocyclic nitrogen compounds	167-253
	100	Heterocyclic oxygen compounds	180	100	Heterocyclic oxygen compounds	180-208
	100	Carboxylic acids	122	100	Carboxylic acids	122
	10	Phenols	94-122	10	Phenols	94-108
				10	Esters	
LC 7	NR			100	Carboxylic acids	122
				100	Heterocyclic nitrogen compounds	129-253
				100	Heterocyclic oxygen compounds	180
				1	Phenols	

(continued)

TABLE C (continued)

c. Sorbent Module Rinses	SASS 1			SASS 2		
	Intensity	Category	MW Range	Intensity	Category	MW Range
LC 1	Nothing detectable			Nothing detectable		
LC 2	10	Fused alt/non-alt hydrocarbons	<216	Nothing detectable		
	1	Fused alt/non-alt hydrocarbons	>216			
	1	Carboxylic acids	256-284			
	4	Esters				
LC 3	100	Fused alt/non-alt hydrocarbons	<216	100	Fused alt/non-alt hydrocarbons	<216
	100	Fused alt/non-alt hydrocarbons	>216	100	Fused alt/non-alt hydrocarbons	>216
	10	Heterocyclic sulfur compounds	184-234	10	Heterocyclic sulfur compounds	234
				1	Sulfur	256
LC 4	100	Fused alt/non-alt hydrocarbons	<216	100	Fused alt/non-alt hydrocarbons	<216
	100	Fused alt/non-alt hydrocarbons	>216	100	Fused alt/non-alt hydrocarbons	>216
	10	Heterocyclic nitrogen compounds	167	10	Heterocyclic nitrogen compounds	167
	10	Heterocyclic sulfur compounds	184-234	10	Heterocyclic sulfur compounds	184
	1	Sulfur	256	1	Sulfur	256
				1	Phenol	94
LC 5	100	Fused alt/non-alt hydrocarbons	<216	100	Fused alt/non-alt hydrocarbons	<216
	100	Fused alt/non-alt hydrocarbons	>216	100	Fused alt/non-alt hydrocarbons	>216
	10	Heterocyclic nitrogen compounds	167	10	Heterocyclic nitrogen compounds	167-217
	10	Heterocyclic sulfur compounds	184, 234	10	Heterocyclic sulfur compounds	184-234
	1	Sulfur	76, 256			
				10	Heterocyclic oxygen compounds	230

(continued)

TABLE C (continued)

c. Sorbent Module Rinses (con.)	SASS 1			SASS 2		
	Intensity	Category	MW Range	Intensity	Category	MW Range
LC 6	100	Heterocyclic nitrogen compounds	153-253	10	Heterocyclic nitrogen compounds	179-253
	100	Heterocyclic oxygen compounds	180-280	10	Heterocyclic oxygen compounds	180-280
	100	Fused alt/non-alt hydrocarbons	<216			
	100	Fused alt/non-alt hydrocarbons	>216			
	10	Carboxylic acids	122			
LC 7	100	Heterocyclic nitrogen compounds	129-253	100	Heterocyclic nitrogen compounds	129-303
				10	Heterocyclic oxygen compounds	180-304
LC 8	NR			10	Heterocyclic nitrogen compounds	129-179
				10	Fused alt/non-alt hydrocarbons	>216
				1	Fused alt/non-alt hydrocarbons	<216
				1	Heterocyclic oxygen compounds	180-230
				1	Phenols	186

APPENDIX D

SUBCATEGORIES, SPECIFIC COMPOUNDS IDENTIFIED IN PHASE 1 ORGANIC EXTRACTS BY LRMS

TABLE D-1. SUBCATEGORIES, SPECIFIC COMPOUNDS IDENTIFIED IN ORGANIC EXTRACTS BY LRMS
(Cyclone Extracts)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
3	Dibenzopyrenes, etc.	302	$C_{24}H_{14}$	-	100
	Methyl dibenzanthracenes, etc.	292	$C_{23}H_{16}$	-	10
	Dibenzanthracenes, etc.	278	$C_{22}H_{14}$	100	100
	Benzoperylene, etc.	276	$C_{22}H_{12}$	100	100
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	100	100
	Methylbenzanthracenes	242	$C_{19}H_{14}$	10	10
	Naphthobenzthiophene	234	$C_{16}H_{10}S$	10	10
	Chrysene, benzanthracenes, etc.	228	$C_{18}H_{12}$	100	100
	Unidentified	218	$C_{17}H_{14}$	10	-
	Benzofluorene	216	$C_{17}H_{12}$	10	-
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	10	-
	Dibenzthiophene	184	$C_{12}H_8S$	10	-
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	10	10
	Biphenyl/acenaphthene	154	$C_{12}H_{10}$	10	-
	Alkyl naphthalenes	142-170	$C_{11}H_{10}$-$C_{13}H_{14}$	10	-
	Naphthalene	128	$C_{10}H_8$	10	-
	Unidentified PAH	200-550		1	1
	Unidentified PAH	258-302		10	
	Unidentified PAH	300-452			10
6	Dioctylphthalate	390	$C_{24}H_{38}O_4$	100	-
	Unidentified	253	$C_{19}H_{11}N$	100	10
	Anthraquinoline, etc.	229	$C_{17}H_{11}N$	100	10
	Unidentified	203	$C_{15}H_9N$	100	10

(continued)

TABLE D-1 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
6	Methyl acridine	193	$C_{14}H_{11}N$	10	10
	Acridine	179	$C_{13}H_9N$	100	100
	Alkyl quinolines	143-171	$C_{10}H_9N$-$C_{12}H_{13}N$	-	1
	Quinoline	129	C_9H_7N	-	1
	Benzoic acid	122	$C_7H_6O_2$	10	1
	Cresol	108	C_7H_8O	1	-
	Phenol	94	C_6H_6O	1	-
	Unidentifiable peaks	100-200			1
	Heterocyclic nitrogen	200-320		10	
	Unidentified heterocyclic	to 400			1
	Unidentified PAH	to 520		1	

TABLE D-2. SUBCATEGORIES, SPECIFIC COMPOUNDS IDENTIFIED IN ORGANIC EXTRACTS BY LRMS (XAD-2 Extract)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
1	Sulfur	256	S_8	NR	100
	Alkanes	to 400	to $C_{30}H_{62}$		10
	Alkenes	to 400	to $C_{30}H_{60}$		10
2	Benzyl naphthalene	218	$C_{17}H_{14}$	10	-
	Benzofluorenes	216	$C_{17}H_{12}$	100	10
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyldibenzthiophene	198	$C_{13}H_{10}S$	-	10
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	100	10
	Dibenzthiophene	184	$C_{12}H_8S$	1	10
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	100
	Alkylbiphenyls/acenaphthenes	168, 182	$C_{13}H_{12}$, $C_{13}H_{14}$	10	10
	Acenaphthene/biphenyl	154	$C_{12}H_{10}$	100	10
	Naphthalene + alkyl napthalenes	128-170	$C_{10}H_8$-$C_{13}H_{14}$	100	10
	Trimethylbenzenes	120	C_9H_{12}	-	10
	Indane/methylstyrene	118	C_9H_{10}	-	10
	Xylene	106	C_8H_{10}	10	10
	Toluene	92	C_7H_8	10	10
	Other PAH	206-246			10
	Other polycyclics	to 300		10	
	Alkylated polycyclics	to 320			1
3	Dibenzopyrenes, etc.	302	$C_{24}H_{14}$	10	-
	Dibenzanthracenes, etc.	278	$C_{22}H_{14}$	10	-
	Dibenzofluorenes, etc.	266	$C_{21}H_{14}$	-	10
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	100	10
	Methyl benzanthracenes	242	$C_{19}H_{14}$	-	10
	Naphthobenzothiophene	234	$C_{16}H_{10}S$	10	10
	Chrysene/benzanthracenes	228	$C_{18}H_{12}$	100	100

(continued)

TABLE D-2 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
3	Benzofluoranthenes	226	$C_{18}H_{10}$	-	100
	Benzylnaphthalene, etc.	218	$C_{17}H_{14}$	100	10
	Benzofluorenes	216	$C_{17}H_{12}$	100	10
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	-	10
	Dibenzthiophene	184	$C_{12}H_{18}S$	1	10
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	100
	Methyl biphenyl/acenaphthene	168	$C_{13}H_{12}$	10	10
	Fluorene	166	$C_{13}H_{10}$	-	10
	Acenaphthylene/biphenyl	154	$C_{12}H_{10}$	100	100
	Acenaphthylene/biphenylene	152	$C_{12}H_8$	-	10
	Naphthalene + alkyl naphthalenes	128-156	$C_{10}H_8$-$C_{12}H_{12}$	100	100-10
	Xylene	106	C_9H_{10}	10	-
	Toluene	92	C_7H_8	10	-
	Other PAH	to 326		10	10
	Other PAH-like material	200-336			1
	Other PAH	to 402		1	
4	Dibenzopyrenes	302	$C_{24}H_{14}$	1	10
	Dibenzanthracenes	278	$C_{22}H_{14}$	1	10
	Benzoperylene, etc.	276	$C_{22}H_{12}$	1	-
	Dibenzocarbazole	267	$C_{20}H_{13}N$	10	10
	Benzpyrenes	252	$C_{20}H_{12}$	10	10
	Methyl chrysene, etc.	242	$C_{19}H_{14}$	-	10
	Naphthobenzothiophene	234	$C_{16}H_{10}S$	-	10
	Chrysene, benzanthracenes, etc.	228	$C_{18}H_{12}$	10	100

(continued)

TABLE D-2 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
4	Benzylnaphthalene, etc.	218	$C_{17}H_{14}$	10	10
	Benzocarbazole	217	$C_{16}H_{11}N$	10	-
	Benzofluorenes	216	$C_{17}H_{12}$	10	10
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyl phenazine/phenanthroline	194	$C_{13}H_{10}N_2$	-	10
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	10	10
	Methyl carbazole	181	$C_{13}H_{11}N$	10	10
	Phenazine/phenanthroline	180	$C_{12}H_8N_2$	-	10
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	100
	Carbazole	167	$C_{12}H_9N$	100	100
	Biphenyl/acenaphthrene	154	$C_{12}H_{10}$	-	10
	Naphthalene + alkylnaphthalenes	128-156	$C_{10}H_8$-$C_{12}H_{12}$	10	10
	Other PAH	200-328		10	10
	Alkyl-substituted polycyclic series	331, 346, 360, 374		-	10
6	Methyl acridine	193	$C_{14}H_{11}N$	100	-
	Fluorenone	180	$C_{13}H_8O$	100	100
	Acridine	179	$C_{13}H_9N$	100	100
	Carbazole	167	$C_{12}H_9N$	-	100
	Benzoic acid	122	$C_7H_6O_2$	100	100
	Methyl cresol	122	$C_8H_{10}O$	1	-
	Cresol	108	C_7H_8O	10	10
	Phenol	94	C_6H_6O	10	10
	Phthalate, not specifically identified			-	10
	Many components, unidentified	200-304		100	
	Major unidentified peak	230			100
	Heterocyclic nitrogen compounds	200-300			10
	Alkyl-substituted polycyclic material	200-500		10	
	Other unidentified material	200-400			1

(continued)

TABLE D-2 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
7	Fluorenone	180	$C_{13}H_8O$	NR	100
	Acridine	179	$C_{13}H_9N$		100
	Carbazole	167	$C_{12}H_9N$		10
	Alkylquinolines	143, 157	$C_{10}H_9N$-$C_{11}H_{11}N$		10
	Quinoline	129	C_9H_7N		10
	Benzoic acid	122	$C_7H_6O_2$		100
	Methyl cresol	122	$C_8H_{10}O$		1
	Cresol	108	C_7H_8O		1
	Phenol	94	C_6H_6O		1
	Unidentified peaks	135-230			100
	Unidentified polycyclic material	280			10

NR - Not reported.

TABLE D-3. SUBCATEGORIES, SPECIFIC COMPOUNDS IDENTIFIED IN ORGANIC EXTRACTS BY LRMS
(Sorbent Module Rinse)

LC	Subcategories, specific compound	m/e	Composition	Intensity SASS 1	Intensity SASS 2
2	Stearic acid	284	$C_{18}H_{36}O_2$	1	Nothing detectable
	Palmitic acid	256	$C_{16}H_{32}O_2$	1	
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	1	
	Chrysene, benzanthracenes	228	$C_{18}H_{12}$	1	
	Benzofluorenes	216	$C_{16}H_{12}$	1	
	Pyrene, etc.	202	$C_{16}H_{10}$	10	
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	1	
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	1	
	Unidentified peak	326		1	
3	Dibenzopyrenes	302	$C_{24}H_{14}$	-	10
	Dibenzanthracenes, etc.	278	$C_{22}H_{14}$	10	10
	Dibenzoperylene/dibenzochrysene	276	$C_{22}H_{12}$	10	10
	Methylcholanthrene, etc.	268	$C_{21}H_{16}$	10	10
	Dibenzofluorenes	266	$C_{21}H_{14}$	10	10
	Sulfur	256	S_8	-	1
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	100	100
	Methyl benzanthracenes, etc.	242	$C_{19}H_{14}$	10	10
	Naphthobenzothiophene/naphtothianaphthene	234	$C_{16}H_{10}S$	10	10
	Chrysene, benzanthracenes	228	$C_{18}H_{12}$	100	100
	Benzyl naphthalene	218	$C_{17}H_{14}$	10	100
	Benzofluorenes	216	$C_{17}H_{12}$	100	100
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	100	100
	Dibenzthiophene	184	$C_{12}H_8S$	10	-
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	100

(continued)

TABLE D-3 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
3	Biphenyl/acenaphthene	154	$C_{12}H_{10}$	10	-
	Naphthalene + alkyl naphthalenes	128-170	$C_{10}H_8$-$C_{13}H_{14}$	10	-
	Carbon disulfide	76	CS_2	-	1
	Other PAH	200-302		10	10
	Other PAH	to 400		1	1
	Alkylated polycyclics	to 430		-	1
4	Dibenzanthracenes, etc.	278	$C_{22}H_{14}$	-	10
	Benzoperylene, etc.	276	$C_{22}H_{12}$	-	10
	Sulfur	256	S_8	1	1
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	100	10
	Naphthobenzothiophene	234	$C_{16}H_{10}S$	10	10
	Unidentified	232		-	10
	Chrysene, benzanthracenes	228	$C_{18}H_{12}$	100	100
	Benzyl naphthalene	218	$C_{17}H_{14}$	100	10
	Benzofluorene	216	$C_{17}H_{12}$	100	10
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	100	10
	Dibenzthiophene	184	$C_{12}H_8S$	10	-
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	100
	Carbazole	167	$C_{13}H_9N$	10	10
	Acenaphthene/biphenyl	154	$C_{12}H_{10}$	10	-
	Acenaphthylene/biphenylene	152	$C_{12}H_8$	10	-
	Alkyl naphthalenes	142-170	$C_{11}H_{10}$-$C_{13}H_{14}$	-	10
	Naphthalene + alkyl naphthalenes	128-170	$C_{10}H_8$-$C_{13}H_{14}$	10	-
	Phenol	94	C_6H_6O	-	1
	Carbon disulfide	76	CS_2	1	-
	Unidentified PAH	258		-	10

(continued)

TABLE D-3 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
4	Unidentified PAH	200-302		10	-
	Unidentified PAH	200-500		1	1
	Alkyl substituted PAH	to 566		1	1
5	Sulfur	256	S_8	1	-
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	100	100
	Methyl chrysene, etc.	242	$C_{19}H_{14}$	-	10
	Naphthobenzothiophene	234	$C_{16}H_{10}S$	10	10
	Benzanthrone	230	$C_{17}H_{10}O$	-	100
	Anthraquinoline	229	$C_{17}H_{11}N$	-	100
	Chrysene, benzanthracenes	228	$C_{18}H_{12}$	100	100
	Benzyl naphthalene	218	$C_{17}H_{14}$	-	100
	Benzocarbazole	217	$C_{16}H_{11}N$	-	10
	Benzofluorenes	216	$C_{17}H_{12}$	100	100
	Heterocyclic nitrogen	203	$C_{15}H_9N$	-	100
	Pyrene, etc.	202	$C_{16}H_{10}$	100	100
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	10	10
	Dibenzthiophene	184	$C_{12}H_8S$	10	10
	Methyl carbazole	181	$C_{13}H_{11}N$	-	10
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	100
	Carbazole	167	$C_{12}H_9N$	10	10
	Carbon disulfide	76	CS_2	1	-
	Other PAH	191-326		10	10
	Other PAH	128-484		-	1
	Alkylated polycyclics	330-468		1	-
6	Dibenzofluorenone	280	$C_{21}H_{12}O$	10	10
	Benzpyrenes, etc.	252	$C_{20}H_{12}$	10	-
	Methyl benzanthrone	244	$C_{18}H_{12}O$	-	10
	Benzanthrone	230	$C_{17}H_{10}O$	100	100

(continued)

TABLE D-3 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
6	Anthraquinoline	229	$C_{17}H_{11}N$	10	-
	Chrysene, benzanthracenes, etc.	228	$C_{18}H_{12}$	100	-
	Benzyl naphthalene, etc.	218	$C_{17}H_{14}$	10	-
	Benzocarbazole	217	$C_{16}H_{11}N$	-	10
	Benzofluorenes	216	$C_{17}H_{12}$	10	-
	Anthraquinone	208	$C_{14}H_8O_2$	10	10
	Pyrene, etc.	202	$C_{16}H_{10}$	100	-
	Methyl fluorenone	194	$C_{14}H_{10}N$	10	-
	Methyl acridine	193	$C_{14}H_{11}N$	10	10
	Methyl anthracene/phenanthrene	192	$C_{15}H_{12}$	10	-
	Dibenzthiophene	184	$C_{12}H_8S$	10	-
	Fluorenone	180	$C_{13}H_8O$	100	100
	Acridine	179	$C_{13}H_9N$	100	100
	Anthracene/phenanthrene	178	$C_{14}H_{10}$	100	-
	Benzoic acid	122	$C_7H_6O_2$	10	-
	Other polycyclics	153-278		10	10
	Other polycyclics	150-304		1	1
7	Anthraquinone	208	$C_{14}H_8O_2$	-	1
	Methyl acridine	193	$C_{14}H_{11}N$	10	10
	Fluorenone	180	$C_{13}H_8O$	-	10
	Acridine	179	$C_{13}H_9N$	100	100
	Alkyl quinolines	143-185	$C_{10}H_9N$-$C_{13}H_{15}N$	100	10
	Quinoline	129	C_9H_7N	100	10
	Unidentified heterocyclic nitrogen compounds	203-253		10	10
	Unidentified heterocyclic oxygen compounds	204-230		-	10
	Unidentified heterocyclic nitrogen compounds	200-303		1	1
	Unidentified heterocyclic oxygen compounds	200-304		-	1
	Unidentified PAH	202-252		10	-

(continued)

TABLE D-3 (continued)

LC	Subcategories, specific compound	m/e	Composition	Intensity	
				SASS 1	SASS 2
8	Benzanthrone	230	$C_{17}H_{10}O$	NR	1
	Chrysene, etc.	228	$C_{18}H_{12}$		1
	Benzyl naphthalene	218	$C_{17}H_{14}$		1
	Benzofluorene	216	$C_{17}H_{12}$		1
	Anthraquinone	208	$C_{14}H_8O_2$		1
	Pyrene, etc.	202	$C_{16}H_{10}$		10
	Methyl fluorene	194	$C_{14}H_{10}O$		1
	Biphenol/phenoxyphenol	186	$C_{12}H_{10}O_2$		1
	Fluorene	180	$C_{13}H_8O$		1
	Acridine	179	$C_{13}H_9N$		1
	Anthracene/phenanthrene	178	$C_{14}H_{10}$		1
	Methyl quinoline	143	$C_{10}H_9N$		10
	Quinoline	129	C_9H_7N		10
	Unidentified peak	163			10
	Other unidentified peaks	200-260			1

APPENDIX E
GRAPHICAL REPRESENTATION
OF PHASE II
IR RESULTS

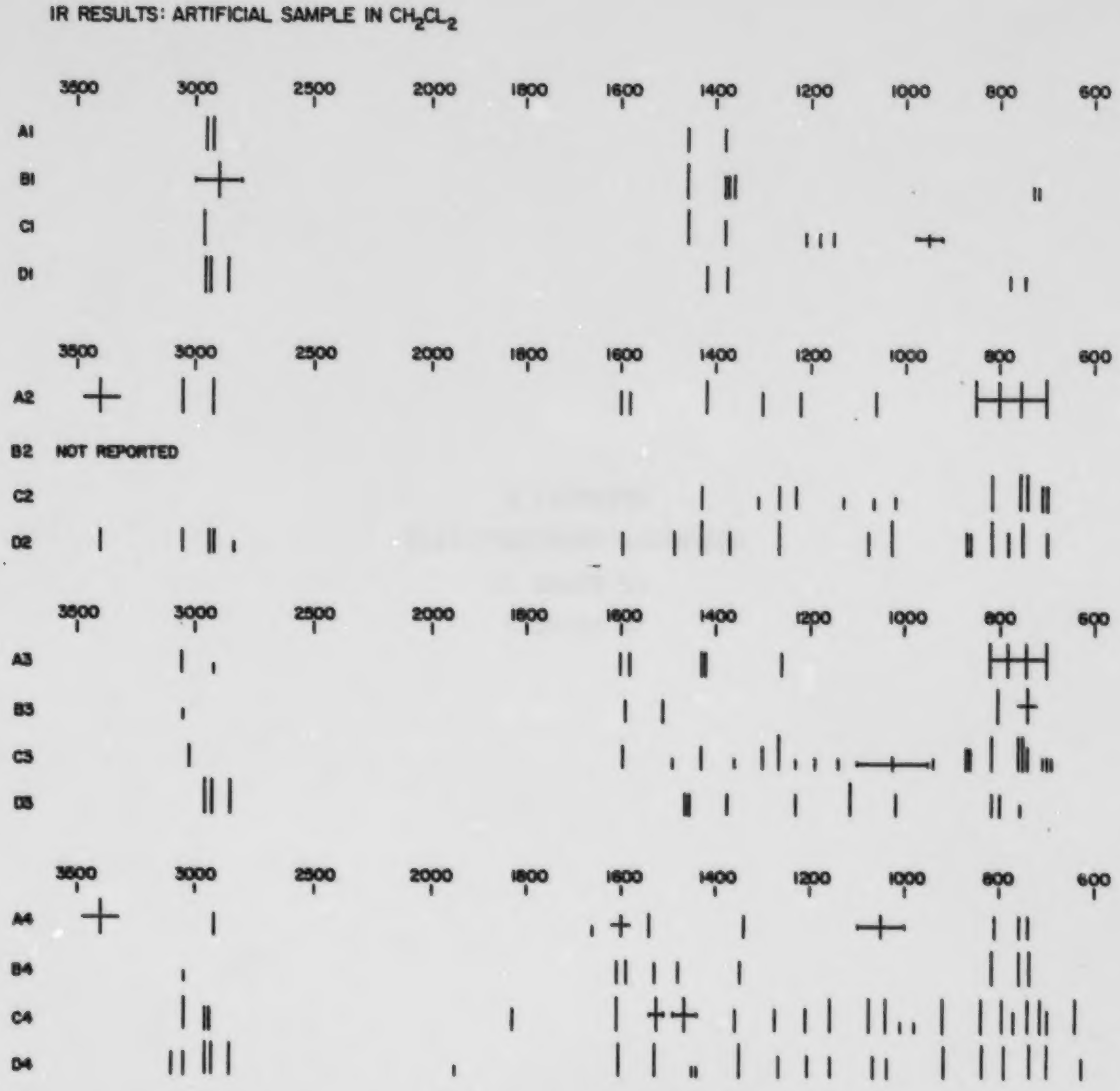


Figure E-1. IR results: artificial sample in CH_2CL_2, LC fractions 1-4.

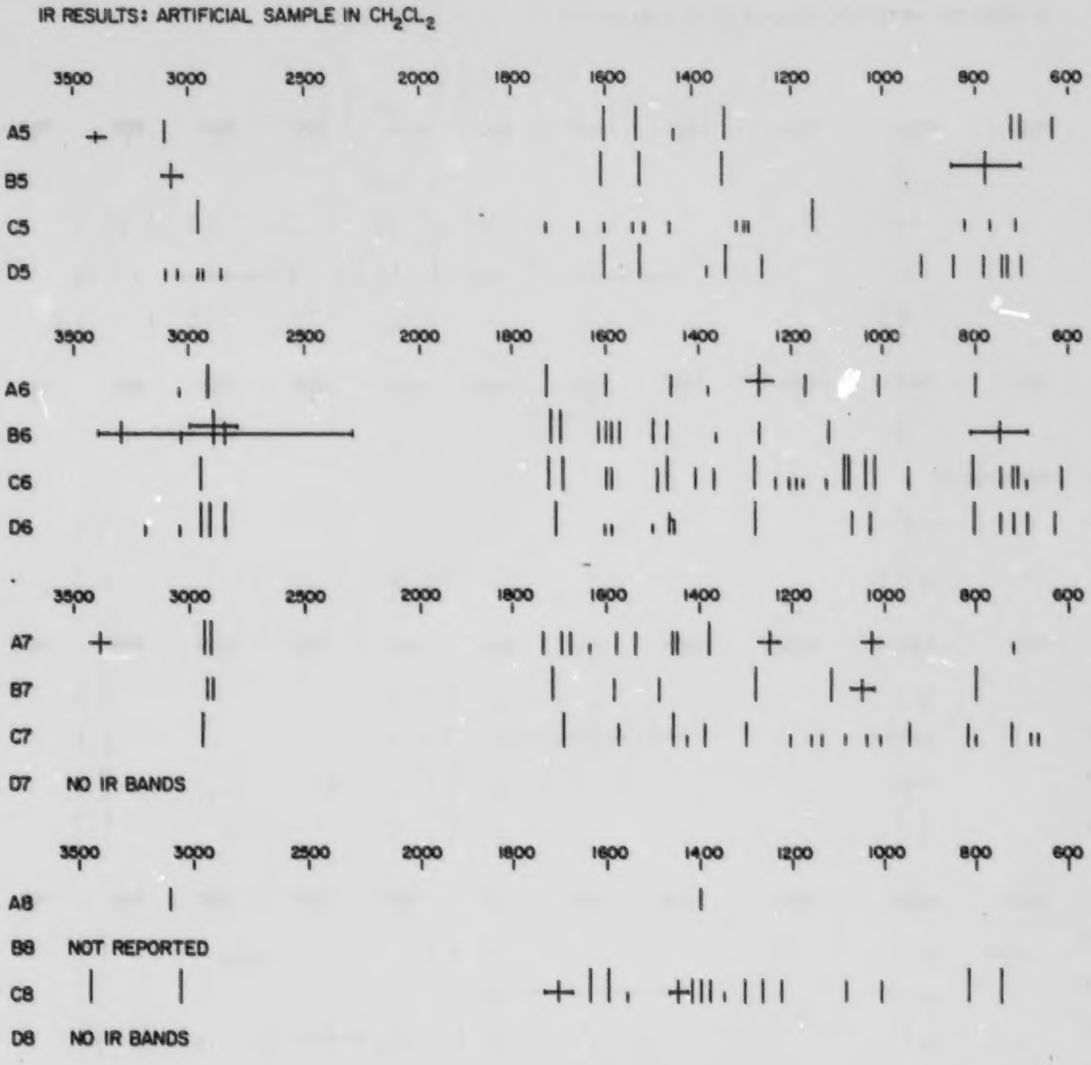


Figure E-2. IR results: artificial sample in CH_2CL_2, LC fractions 5-8.

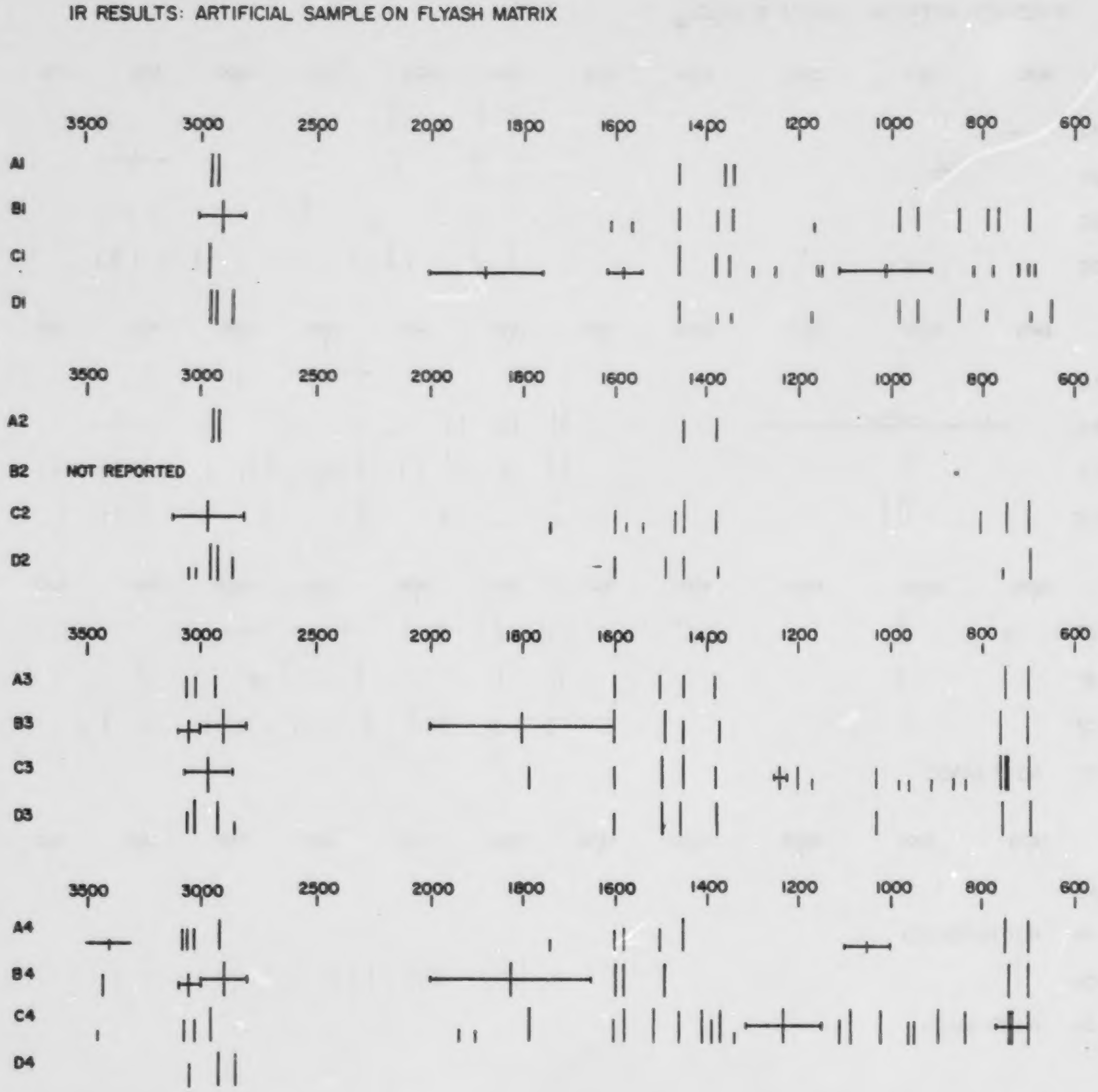


Figure E-3. IR results: artificial sample on flyash matrix, LC fractions 1-4.

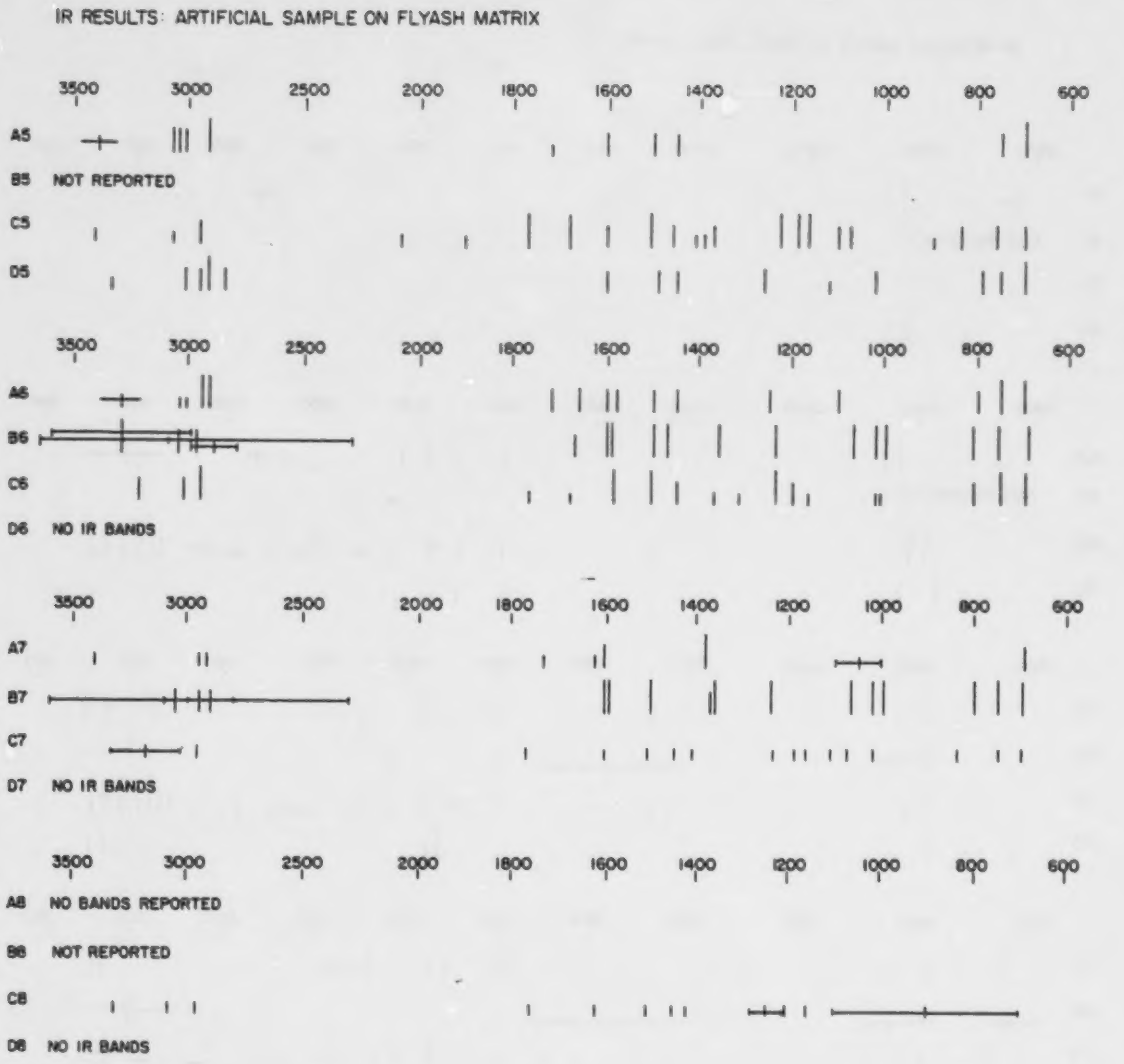


Figure E-4. IR results: artificial sample on flyash matrix, LC fractions 5-8.

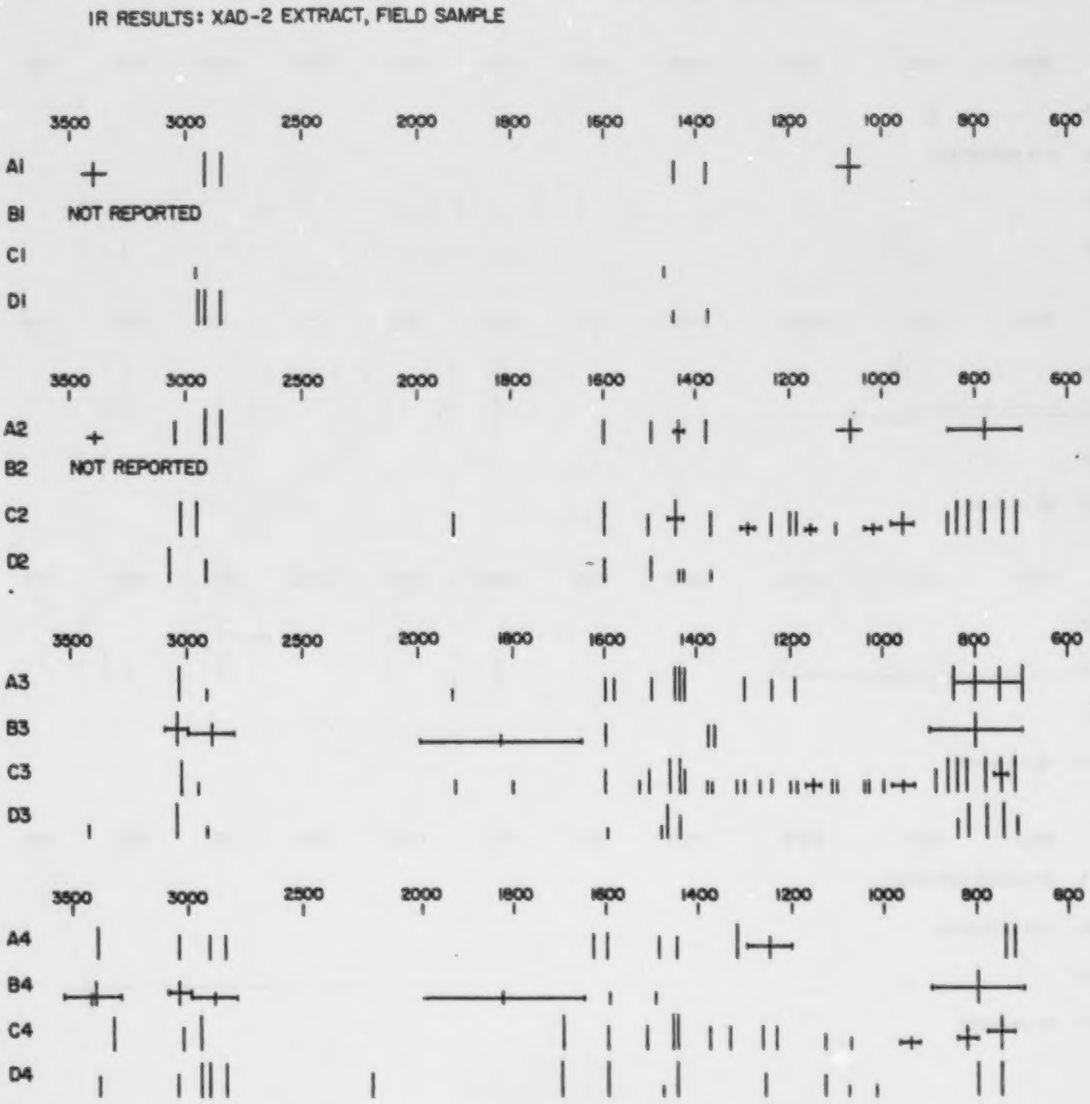


Figure E-5. IR results: XAD-2 extract, field sample, LC fractions 1-4.

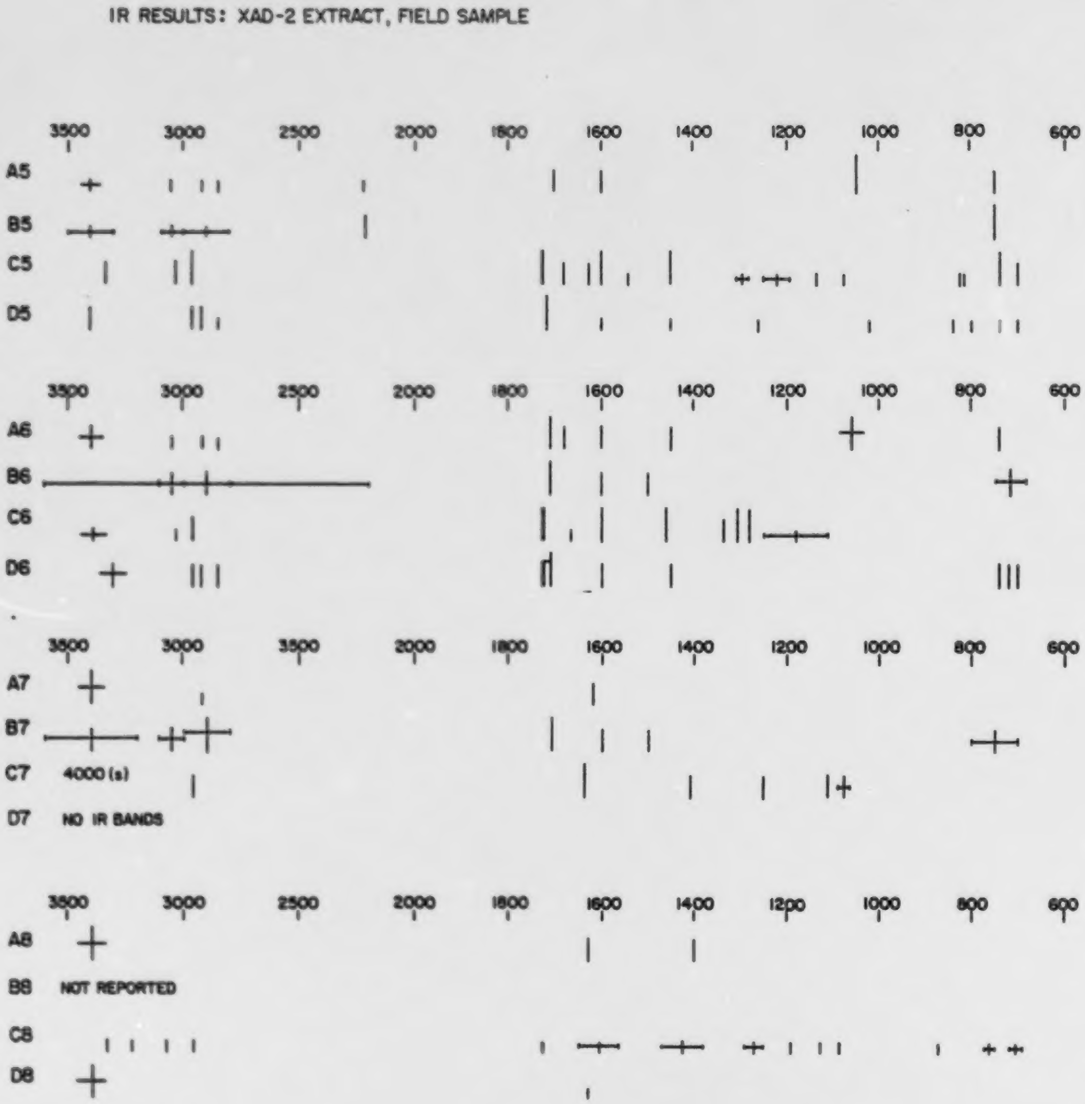


Figure E-6. IR results: XAD-2 extract, field sample, LC fractions 5-8.

APPENDIX F
PHASE II
IR RESULTS:
LC FRACTIONS

TABLE F-1. IR RESULTS: ARTIFICIAL SAMPLE IN CH_2CL_2, LC FRACTIONS

	A			B		
LC1	2,920, 2,950	S	saturated CH	3,000-2,800	S	CH, aliphatic
	1,460	M	CH_3, CH_2	1,460	S	CH, aliphatic
	1,380	M	CH_3	1,380, 1,372, 1,360	M	$C\text{-}CH_3$
				729, 718	W	CH_2; $-(CH_2)n-$, N ≥ 4
LC 2	3,400	S (v broad)	OH, NH	NR		
	3,050	S	unsaturated CH			
	2,920	S	saturated CH			
	1,600, 1,580	M	ring vibrations			
	1,420	S (sharp)	CH_2, $S\text{-}CH_3$			
	1,300	M	$S\text{-}CH_3$, $CH_2C\ell$			
	1,220	M	phenol			
	1,060	M	alcohol; subs. arom.			
	700-850	S (multiple)	subs. arom.; fused ring compds; $C\text{-}C\ell$ (740 cm^{-1})			

(continued)

TABLE F-1 (continued)

	C			D		
LC1	2,960	S	CH_2	2,950, 2,930, 2,855	S	aliphatic CH
	1,460	S	CH_3	1,420	M	alkanes
	1,380	M	isopropyl	1,375	M	alkanes
	1,210	W	$=CH_2$ in plane	780, 745	W	halogens
	1,180	W	isopropyl			
	1,150	W	$-CH=CH_2$			
	980-920	W	cyclohexane derivative			
	730	W	$-CH_3$ or $C\text{-}C\ell$			
LC 2	1,430	M	$C=CH_2$	3,400	M	OH (water)
	1,310	W	C=C trans	3,050	M	aromatic CH
	1,265	M	$C\text{-}CH_2$ (possibly in ring)	2,940, 2,920	M	aliphatic CH
	1,230	M	aromatic substitution	2,835	W	aliphatic CH
	1,130	W		1,595, 1,485	M	aromatic ring
	1,065	W		1,430	S	alkenes
	1,020	W		1,370	M	alkanes, alcohols
	815	S		1,265	S	aromatic ethers
	755	S		1,075	M	alcohols, aromatic overtones
	740	S		1,025	S	aromatic ether, aromatic overtones
	710	M		870, 860, 780, 695	M	aromatic substistution
	700	M		815, 750	S	aromatic substitution

(continued)

TABLE F-1 (continued)

	A			B		
LC3	3,050	M	unsaturated CH	~3,045	W	CH, aromatic
	2,920	W	saturated CH	1,590, 1,510	M	C=C, aromatic
	1,600, 1,580	M	ring vibrations	812, 760-720	S	ϒ(CH), aromatic
	1,420, 1,430	M	aromatic CH, CH_2, $CH_2C\ell$			
	1,260	M	oxirane, $CH_2C\ell$			
	700-820	S (multiple)	Subs. arom. or fused ring compds.			
LC4	3,400	S(braod)	OH, NH	3,050	W	CH, aromatic
	2,920	M	saturated CH	1,610, 1,590, 1,480	M	C=C, aromatic
	1,720	W	dialkylketone, esters, imide, carbonate	1,530, 1,348	M	NO_2
	1,600	M (somewhat broad)	ring vibrations, C=C	815, 760, 734	S	ϒ(CH), aromatic
	1,540	M	NO_2			
	1,340	M	aryl NH^-, NO_2			
	1,000-1,100	M (broad)	C-O, alcohol, ether, ester			
	810, 740, 760	M	arom. subs., fused rings, subs. pyridine			

(continued)

TABLE F-1 (continued)

	C			D		
LC3	3,020	M	aromatics	2,960, 2,930, 2,855	S	aliphatic CH
	1,595	M	aromatics	1,465, 1,455	M	aliphatics
	1,490	W	aromatics	1,375	M	alkanes
	1,430	M	$C=CH_2$	1,260	M	aromatic ethers, esters
	1,360	W	$C(CH_3)x$	1,115	S	aliphatic ethers
	1,300	M	C=C trans	1,020	M	primary alcohols, aromatic ethers
	1,265	S	cyclohexyl derivative	815, 800	M	alkenes
	1,230	W		755	W	halogen
	1,190	W	(possibly pyridine)			
	1,140	W	aromatics			
	1,100-950	W	cyclohexyl derivative			
	940	W				
	870, 860	M	benzene derivatives; C-Cℓ at 740			
	815	S				
	760, 750	S				
	740	M				
	710, 700, 690	W				
LC4	3,050	S	aromatic C-H	3,100, 3,050	M	aromatic CH
	2,960	M	$-CH_2$	2,960, 2,930, 2,855	M	aliphatic CH
	2,940	M	aromatic or β-lactone	1,950	W	aromatic overtones, C=C=C
	1,830	M	aromatic	1,605	S	aromatic ring, amines
	1,610	S	aromatic or $ArNO_2$	1,530	S	broad, aromatic ring
	1,540-1,510	S	$-CH_2$	1,450, 1,440	W	alkanes
	1,490-1,440	S	$ArNO_2$	1,350	S	alcohols
	1,360	M		1,265	M	aromatic alcohols, aromatic ethers, esters
	1,275	M	Tert-butyl benzene	1,205	M	aromatic ethers, phenols
	1,210	M		1,155	M	aliphatic ethers, phenols amines, aromatic overtones

(continued)

TABLE F-1 (continued)

	C			D		
LC4	1,160	S	$(CH_3)_2C$	1,065, 1,035	M	aromatic ethers, aliphatic alcohols, aromatic overtones
	1,075	S		915	S	alkenes
	1,040	S	aromatic substitution	835, 790, 735, 700	S	aromatic subst.
	1,010	W		625	M	alkenes, halogens
	980	W		3,400, 2,740, 1,730, 1,690		weak peaks
	920	S	CH=CH2			
	840	S	$>C=CH_2$			
	795	S	$(CH_3)_2C$			
	770	M				
	740	S	aromatic substitution			
	715	S				
	700	M				
	640	S	C-Cℓ			

(continued)

TABLE F-1 (continued)

	A			B		
LC5	3,400	W (broad)	OH, NH	3,110-3,030	M	CH, aromatic
	3,100	M	unsaturated CH	1,607	S	C=C, aromatic
	1,600	S	ring vibration	1,525, 1,345	S	NO_2
	1,530	S	$-NO_2$	850-700	S	T(CH), aromatic
	1,450	W	CH_2			
	1,340	S	$-NO_2$			
	700, 720	M	arom. substitution			
	630	M	monoalkyl (benzene, alkylnaphthalene)			

(continued)

TABLE F-1 (continued)

	C			D		
LC5	2,960	S	CH stretch	3,100, 3,050	W	aromatic CH
	1,725	S	C=0	2,960, 2,940, 2,860	W	aliphatic CH
				1,600	S	aromatic rings, amides
	1,600	M	benzene substitution	1,525	S	aromatic rings, amides
	1,540	S	CNO_3	1,380	W	alcohols
	1,350	S	$ArNO_x$ or COO^- or aldehyde	1,340	S	alcohols, amines, amides
	1,290	S	aldehyde, benzoate, nitroaldehyde or ketone	1,260	M	phenols, esters
	1,135-1,110	M	PhCOR, phthalate	915	M	alkenes, alcohols, carboxylic acids
	1,075	M		845, 780, 740, 730, 700	M	aromatic substitution
	1,040	W	aromatics	1,200, 1,150, 1,125, 1,070, 1,030		weak peaks
	1,020	W				
	835	W	aldehyde, >C=CH			
	820	M				
	795	W				
	760	M	aromatics			
	730	W				
	705	M				
	680	M	C-Cℓ			

(continued)

TABLE F-1 (continued)

	A			B		
LC6	3,050	W	unsaturated CH	3,400-2,300	M	OH, acidic
	2,920	S	saturated CH	3,300	M	OH, alcoholic
	1,730	S	C=O, ester, ketone, imide, carbamate	3,040	W	CH, aromatic
	1,600	M	ring vibrations	3,000-2,800	S	CH, aliphatic
	1,460	M	CH_2, CH_3, S-CH_2	1,720, 1,700	S	C=O, ester and acid
	1,380	W	CH_3	1,618, 1,602, 1,590, 1,572, 1,498	M	C=C, aromatic
	1,270	S (broad)	$CH_2Cℓ$, C-O, S-CH_2, ether, ester, S-CH_3	1,270, 1,120	M	C-O-C, aromatic ester
	1,170	M	ester	1,469	M	CH, aliphatic
	1,010	M	alcohol, arom. subs.	1,362	W	C-CH_3
	800	M	R_2C=CHR, S-CH_3	810-690	M	Υ(CH), aromatic
				1,100		minor absorption maximum

(continued)

TABLE F-1 (continued)

	C			D		
LC6	2,960	S	C-H stretch	3,200	W	broad, -OH
	1,725	S	C=0	3,050	W	aromatic CH
	1,600, 1,590	W	aromatic	2,960, 2,920 2,850	S	aliphatic CH
	1,490	M	aromatics (nitro compound)	1,710	S	carbonyls
	1,470	M	$-C-CH_3$	1,605, 1,590, 1,500	W	aromatic ring
	1,450	W	$-CH_2$-possibly in ring	1,465, 1,455 (sh)	M	aliphatic CH, carboxylic acids
	1,410	W	$-C=CH_2$	1,280	S	sulfonic acids, silica
	1,370	M	$-C-CH_3$	1,070, 1,030	M	sulfoxides, aromatic overtones
	1,290	S	C=0	805	S	aromatic substitution
	1,205, 1,175	W	=CH in plane bend, phthalate, benzoate	750, 720, 690	M	aromatic substitution
	1,125	M	=CH in plane bend	630	M	S-0
	1,085	M	S=0 stretch or phthalate or cyclohexyl compound	1,410, 1,370, 1,225, 1,120, 1,090, 1,010, 940, 780		weak peaks
	1,075	M	S=0 stretch			
	1,045	M	S=0 stretch or =CH in plane bend			
	1,020	M	acid or cyclohexyl derivative			
	945	W				
	805	M	aromatics			
	745	M				
	720	W				
	710	W				
	625	m	C-S			

(continued)

TABLE F-1 (continued)

	A			B		
LC7	3,400	M	OH, NH	2,910, 2,840	M	CH, aliphatic
	2,920, 2,950	S	saturated CH	1,722	S	C=0, aromatic ester
	1,740	M	cyclic ketone, esters	1,585, 1,488	M	C=C, aromatic
	1,700	M	conj. ketone, acid, imide, carbamate	1,280, 1,115	S	C-0-C, aromatic ester
	1,680	M	ketones, amide	1,100-1,000	M	C-0
	1,640	W	amide, C=C	802	S	Υ(CH), aromatic
	1,580	M	NO_2, $CHC\ell NO_2$			
	1,540	M	C-N=0, NO_2			
	1,450, 1,460	M	CH_2, CH_3			
	1,380	S	CH_3, NO_2			
	1,250	M (broad)	phenol, ether, ester			
	1,030	M (broad)	C-0, alcohol, ether, subs. arom.			
	720	W	subs. arom.			

(continued)

TABLE F-1 (continued)

	C			D
LC7	2,960	S	C-H stretch	no IR bands
	1,695	S	C=0: aldehyde, ketone or acid	
	1,575	M	COO^-	
	1,460	S	$-CH_2$	
	1,430	W	acid or aldehyde	
	1,390	M	$>C=CH_2$	
	1,300	M	C-0 stretch	
	1,205	W	=CH in plane bend	
	1,160	W		
	1,135	W		
	1,085	W	aromatics	
	1,040	W		
	1,010	W		
	945	M	acid	
	820	M	aromatics	
	805	W		
	725	M		
	685	W		
	665	W	C=C	

(continued)

TABLE F-1 (continued)

	A			B
LC8	3,100		ammonium salt	NR
	1,400		ammonium salt	
	C			D
LC8	3,450	S	water	no bands
	2,960	S	C-H stretch	
	1,740-1,680	M	C=0	
	1,640	S	water	
	1,600	S	aromatic or COO^-	
	1,560	W	aromatic	
	1,470-1,430	M	$C-CH_3$	
	1,420	M	$-C=CH_2$	
	1,400	M	$-C-(CH_3)_3$	
	1,380	M		
	1,350	W	aldehyde or COO^-	
	1,305	M	aldehyde, acid, or C=C trans	
	1,265	M	CH_2	
	1,225	M	$C-(CH_3)_3$	
	1,085	M	alcohol, acid or aromatic	
	1,010	M	aromatics	
	820	S		
	750	S		

TABLE F-2. IR RESULTS: ARTIFICIAL SAMPLE ON FLYASH MATRIX, LC FRACTIONS, ALIQUOT 1

	A			B		
LC1	2,920, 2,950	S	aliphatic CH	3,000-2,800	S	CH, aliphatic
	1,460	M	CH_2, CH_3	1,605, 1,560, 1,165	W	1,3 hexachlorobutadiene
	1,340, 1,360	M	CH_3, CH_2	1,460	M	CH, aliphatic
				1,375	M	C-CH
				1,342, 698	M	hexachlorobenzene
				980, 940, 850, 790, 765	M	1,3-hexachlorobutadiene
				720		minor absorption maximum
LC 2	2,920, 2,950	S	aliphatic CH	Not reported		
	1,450	M	CH_2, CH_3			
	1,380	M	CH_3			

(continued)

TABLE F-2 (continued)

	C			D		
LC1	2,960	S	C-H stretch	2,955, 2,925, 2,855	S	aliphatic CH
	2,000-1,755 1,615-1,540	W	aromatic	1,460	M	alkanes
				1,375, 1,345, 1,170	W	alkanes, alkenes
				980, 940	M	alkanes, alkenes
	1,460	S	-CH_2	850	M	alkenes
	1,380, 1,350	M	-$C(CH_3)_x$	190, 695	W	not aromatic substitution, possible halogens
	1,300, 1,250, 1,155, 1,150	W	aromatics	650	M	
	1,110-910	W	phosphate	1,560	weak peak	
	820, 775, 720, 700	W	aromatics			
	685	W	C-Cℓ			
LC2	3,125-2,815	S	aromatics	3,055, 3,020	W	aromatic CH
	1,740	W	C-H stretch	2,960, 2,930	S	aliphatic CH
	1,600	M	aromatics	2,860	M	aliphatic CH
	1,575	W		1,600, 1,490	M	aromatic ring
	1,540	M		1,450	M	aliphatics
	1,470	M	-$C(CH_3)_x$	1,375	W	aliphatics
	1,450	S		755	W	aromatic substitution
	1,380	M		695	S	aromatic substitution
	805	M	aromatics	1,025	weak peak	
	750	S				
	700	S				

(continued)

TABLE F-2 (continued)

	A			B		
LC3	3,020, 3,060	M	unsaturated CH	3,100-3,000	M	CH, aromatic or olefinic
	2,930, 2,950	M	saturated CH	3,000-2,800	S	CH, aliphatic
	1,600	M	ring vibrations	2,000-1,600, 1,598, 1,490, 758, 697	S	monosubstituted benzene
	1,500	M	ring vibrations	1,450	M	CH, aliphatic
	1,450	M	CH_2	1,370	M	$C-CH_3$
	1,380	M	CH_3	735		minor absorption maximum
	700, 750	S (sharp)	subs. aromatic, fused ring compounds			
LC4	3,400	W (broad)	OH, NH	3,425	M	NH, secondary amine
	3,030, 3,060, 3,080	M	unsaturated CH	3,100-3,000	M	CH, aromatic
	2,920	S	saturated CH	3,000-2,800	S	CH, aliphatic
	1,600, 1,580, 1,500	M	ring vibrations	2,000-1,650, 1,596, 1,578, 1,489, 740, 697	S	monosubstituted benzene
	1,450	S (sharp)	CH_2	757		minor absorption maximum
	1740	W	cyclic ketone, α Cℓ ketone, ester			
	1,000-1,100	W (broad)	C-O, ester, alcohol			
	750, 700	S	subs. arom; fused ring compounds			

(continued)

TABLE F-2 (continued)

	C			D		
LC3	3,075-2,860	S	aromatics and C-H	3,060	M	aromatic CH
	1,785	M	aromatic, $>C=CH_2$	3,025	S	aromatic CH
	1,600	M	aromatic	2,925	S	aliphatic CH
	1,495	S	aromatic	2,850	W	aliphatic CH
	1,450	S	$-CH_2-$ and $(CH_3)_3C$	1,600	M	aromatic ring
	1,380	M	$-(CH_3)_3C$	1495	S	aromatic ring
	1,250-1,225	M	$-(CH_3)_3C$	1,455, 1,375	S	aliphatics
	1,200	M		1,030	M	aromatic overtones
	1,170	W		755	S	aromatic substitution
	1,030	M		695	S	aromatic substitution
	980, 960	W				
	910, 860	W	aromatics			
	835	W				
	760	S				
	750, 745	S				
	700					
LC4	3,450	W	OH or NH	3,050	M	aromatic CH
	3,075, 3,030	M	aromatics	2,925, 2,850	S	aliphatic CH
	2,960	S	C-H stretch			
	1,940, 1,905	W	aromatics			
	1,785	S	$>C=CH_2$, acid chloride, carbonate or lactone			
	1,600	M	aromatic			
	1,515	S	aromatic, $C-NO_x$, NH_4 CIR, $NH_4C\ell R$, NH_4 + or phenol			
	1,460	S	$(CH_3)_x$ C			
	1,410	S	$>C=CH_2$			
	1,390	M	$C(CH_3)_3$			
	1,370	S	C=C (trans)			

(continued)

TABLE F-2 (continued)

	C			D
LC4	1,340	W	phenols, ethers, or sulfonic acids	
	1,315-1,150	S	aromatic	
	1,110	M	sulfonic acid	
	1,085	S	aromatics: pyridines, phenols	
	1,020	S	$>C=CH_2$, phenols, or pyridines	
	960, 945	M		
	895	S		
	835	S		
	770-700	S	aromatics	
	740	S		
	700	S		

(continued)

TABLE F-2 (continued)

	A			B
LC5	3,400	W (broad)	OH, NH	Not reported
	3,020, 3,050, 3,080	M	unsaturated CH	
	2,920	S	saturated CH	
	1,720	W	cyclic ketone, αCℓ ketone, ester	
	1,600	M	ring vibrations	
	1,500	M	ring vibrations	
	1,450	M	CH_2	
	700	S (sharp)	arom. or fused rings	
	750	M	subs. arom., fused rings, C-Cℓ	

(continued)

TABLE F-2 (continued)

	C			D		
LC5	3,415	W	NH or OH	3,340	W	N-H, -OH
	3,075	W	aromatic	3,020	M	aromatic CH
	2,960	M	C-H stretch	2,960, 2,850	M	aliphatic CH
	2,085	W	C=C or nitrile	2,920	S	aliphatic CH
	1,905	W	aromatic	1,600	M	aromatic ring, amines
	1,770	S	C=CH_3, carbonate, acid chloride, lactone	1,490	M	aromatic ring
	1,680	W	aldehyde, ketone, or acid	1,450	M	aliphatics
	1,600	M	aromatic	1,260	M	aromatic ethers, COOH
	1,505	S	aromatic, C-NO_x, $NH_4C\ell R$, NH_4^+, phenols	1,120	W	aliphatic ethers, amines
	1,460	M	$C(CH_3)_3$	1,020	M	aromatic overtones, aromatic ethers, amines
	1,410, 1,390	W	>C=CH_2	790, 750	M	aromatic substitution
	1,370	M	$C(CH_3)_3$	695	S	
	1,225, 1,190	S	phenols, ethers, sulfonic acids			
	1,165	S	aromatic			
	1,100	M	sulfonic acid			
	1,075	M	pyridines, phenols			
	1,015	S	C=CH_2, phenols			
	895	W	aromatics			
	835, 760, 700	M				

(continued)

TABLE F-2 (continued)

	A			B		
LC6	3,300	W (broad)	NH, C=CH, NH_4^+	3,650-2,300	M	OH, acidic
	3,020, 3,050	W	unsaturated CH	3,600-3,000	S	OH, alcoholic or phenolic
	2,920, 2,950	S	saturated CH	3,100-3,000	M	CH, aromatic
	1,720	M	cyclic ketone, $\alpha C\ell$ ketone, ester	3,000-2,800	W	CH, aliphatic
	1,660	M	ketones, mono subs. amide, C=N, >C=CH, CH_2ONO	1,668	M	C=0, amide I, or C=C olefinic
	1,600, 1,580	M	ring vibrations	1,602, 1,592, 1,498, 1,470, 753, 690	S	monosubs. benzene
	1,500	M	ring vibrations	1,360, 1,235, 1,068, 1,021, 997, 810, 753 690	S	phenol
	1,450	M	CH_2			
	1,250	M	$^{O}\diagdown_{N}{=}\,^{N}\diagdown_{O}$, phenol, arom. ether, ester, $CH_2C\ell$, CH_2Br			
	1,100	M (broad)	alcohol, aliphatic ester, ester			
	800	M	CH_2-0-NO			
	750, 700	S	$CH_2C\ell$, $CC\ell_3$, cyclic C-$C\ell$, arom. subs. or fused ring compounds			

(continued)

TABLE F-2 (continued)

	C			D
LC6	3,225	M	N-H or OH	No IR bands
	3,030	M	aromatic	
	2,960	S	C-H stretch	
	1,770	W	$C=CH_2$, acid chloride, carbonate or lactone	
	1,680	W	aldehydes, ketone, or acid	
	1,585	S	aromatic	
	1,505	S	aromatic, $C-NO_x$, $NH_4C\ell$ or NH_4†, phenols	
	1,450	M	$C(CH_3)_x$	
	1,370	W	$C(CH_3)_3$	
	1,315	W	C=C (trans)	
	1,235	S	phenols, ethers, or sulfonic acids	
	1,200	M		
	1,165	W		
	1,020	W	aromatics, especially pyridines and phenols	
	1,010	W		
	805	M	aromatics	
	750	S		
	695	S		

(continued)

TABLE F-2 (continued)

	A			B		
LC7	3,400	W	OH, NH	3,600-2,300	M	OH, acidic
	2,920, 2,950	W	saturated CH	3,100-3,000	M	CH, aromatic
	1,730	W	cyclic ketone αCℓ ketone, ester	3,000-2,800	M	CH, aliphatic
	1,620	W	C=C	1,600, 1,590, 1,500, 1,360, 1,240, 1,065, 1,020, 995, 803, 750, 695	S-M	phenol
	1,600	M	ring vibrations, SiCH=CH_2			
	1,380	S	SiCH=CH_2, inorganic salt?	1,369	M	C-CH_3
	1,000-1,100	W (broad)	C-O	1,720, 1,670, 780		minor absorption maxima
	690	M	subs. arom.			
LC8	Ammonium salt (chloride)			Not reported		

(continued)

TABLE F-2 (continued)

	C			D
LC7	3,335-3,030	W	NH or OH and aromatics	No IR bands
	2,960	W	C-H stretch	
	1,770	W	$C=CH_2$, acid Cl, carbonate or lactone	
	1,600	W	aromatics	
	1,505	W	aromatics, CNO_x, NH_4+ compound or phenols	
	1,450	W	$C(CH_3)_x$	
	1,410, 1,235, 1,190, 1,165	W	phenols, ethers sulfonic acids	
	1,110, 1,075, 1,020, 835, 750, 700	W	aromatics	
LC8	3,335	W	NH or OH	No IR bands
	3,075	W	aromatics	
	2,960	W	C-H	
	1,755	W	C=0	
	1,615	W	aromatics	
	1,505	W	aromatics, $C-NO_x$, NH_4+	
	1,450, 1,420	W	$C(CH_3)_3$	
	1,280-1,210, 1,205, 1,163	W	phenols and sulfonic acids	
	1,110-700	W	aromatics	

TABLE F-3. IR RESULTS: FIELD SAMPLE, XAD-2 EXTRACT, RUN 1, LC FRACTIONS

	A			B
LC1	3,400	M (broad)	OH, NH	Not reported
	2,850, 2,920	S	saturated CH	
	1,450	M	CH_2, CH_3	
	1,380	M	CH_3	
	1,070	S (broad)	SiO-aliphatic, alcohol, Si-O-Si	
LC 2	3,400	W (broad)	OH, NH	Not reported
	3,050	M	unsaturated CH	
	2,850, 2,920	S	saturated CH	
	1,600	M	ring vibrations	
	1,500	M	ring vibrations	
	1,430-1,450	M	$CH_2C\ell$, CH_2Br, CH_2, CH_3	
	1,380	M	CH_3	
	1,070	M (broad)	Si-O-aliphatic, Si-O-Si	
	700-860	M	Subs. arom. or fused ring compounds	

(continued)

TABLE F-3 (continued)

	C			D		
LC1	2,960	W	C-H	2,950, 2,920 2,850	S	aliphatic CH
	1,470	W	$C(CH_3)_x$	1,450	W	alkanes
	715	W	aromatic	1,375	W	alkanes
				1,530	weak peak	
LC2	3,030	S	aromatics	3,040	S	aromatic CH
	2,960	S	C-H stretch	2,920	M	aliphatic CH
	1,925	M		1,600, 1,500	M	aromatic ring
	1,600	S	aromatics	1,455	S	alkanes
	1,505	M		1,440, 1,430, 1,370	W	aliphatics
	1,460-1,430	S	C=C	1,240, 1,185	M	aromatic overtones
	1,370	M	$C(CH_3)_3$	1,140, 1,090	W	aromatic overtones
	1,305-1,275	W	$C(CH_3)_3$	845, 815, 780, 745, 735, 710	S	aromatic substitution
	1240	M	C-Cℓ	1,925, 1,670, 1,300, 865	weak peaks	
	1,200, 1,185	M	aromatic			
	1,165-1,143	W	aromatics or $C(CH_3)_3$			
	1,100	W	aromatic			
	1,040-1,000	W	aromatics			
	980-935	M	cyclohexanes			
	860	M	aromatic substitution			
	840, 815, 780, 740, 710	S	C-Cℓ			

(continued)

TABLE F-3 (continued)

	A			B		
LC3	3,040	S	unsaturated CH	3,100-3,000	S	CH, aromatic
	2,920	W	saturated CH	3,000-2,800	M	CH, aliphatic
	1,930	W (broad)	alkene	2,000-1,650	W	combination bands, aromatic rings
	1,600, 1,580	M	ring vibrations	1,597, 1,596	M	C=C, aromatic
	1,500	M (sharp)	ring vibrations	1,376, 1,364	M	C-CH_3
	1,450	S	CH_2, CH_3	900-700	S	Υ(CH), several aromatic rings
	1,440		S-CH_3			
	1,430		aromatic CH			
	1,300	M	S-CH_3			
	1,240	M	S-CH_2			
	1,190	M	subs. arom.			
	700 (850)	S (multiple-sharp)	Subs. aromatic or fused ring compounds, subs. pyridines			
LC4	3,400	S	NH, OH	3,415	M	NH, secondary amine
	3,050	M	unsaturated CH	3,550-3,300	W	OH, alcoholic
	2,850, 2,920	M	saturated CH	3,100-3,000	M	CH, aromatic
	1,630	M	C=C	3,000-2,800	W	CH, aliphatic
	1,600, 1,490	M	ring vibrations	2,000-1,650	W	combination bands aromatic rings
	1,450	M	CH_2, CH_3	1,595, 1,495	W	C=C, aromatic
	1,200-1,300	M (v broad)	aryl or vinyl ether	900-700	S	Υ(CH), several aromatic rings
	720, 740	S (sharp)	subs. arom. or fused ring compounds			

(continued)

TABLE F-3 (continued)

	C			D		
LC3	3,030	S	aromatics	3,430	W	OH, N-H
	2,960	W	C-H stretch	3,050	S	aromatic CH
	1,925, 1,800	W		2,920	W	aliphatic CH
	1,600	M	aromatic	1,595, 1,480	W	aromatic ring
	1,525	W		1,465	S	aliphatic
	1,505	M		1,440	M	aliphatic, alkenes
	1,460, 1,440	S	$C(CH_3)_x$, C=C	815, 775, 740	S	aromatic
	1,430	M		840, 710	M	substitution
	1,380, 1,370	W	$C(CH_3)_3$	1,265	weak peak	
	1,315, 1,300, 1,265, 1,240, 1,200, 1,185, 1,165-1,135, 1,110, 1,100, 1,040, 1,030, 1,000, 980-928	W	aromatics			
	885	M	aromatics			
	860, 840	S				
	820, 780, 760-730, 715	S	aromatics C-Cℓ			
LC4	3,335	S	OH or NH	3,400	M	-NH, -OH
	3,030	M	Aromatics	3,060	M	aromatic CH
	2,960	S	C-H stretch	2,960, 2,920 2,850	S	aliphatic CH
	1,695	S	aldehyde or ketone	2,220	M	nitriles
	1,600, 1,515	M	aromatics	1,700	S	carbonyls
	1,460, 1,450	S	$C(CH_3)_x$	1,600	S	broad, aromatic ring, amines, amide, carboxylic acid

(continued)

TABLE F-3 (continued)

	C			D		
LC4	1,380	M	$C(CH_3)_2$	1,480	W	aromatic ring
	1,335	M	C=C	1,450	S	broad, alkanes
	1,265, 1,235	M	$C(CH_3)_3$	1,260	M	aromatic ether, phenols, carboxylic acids, esters
	1,130, 1,075, 970-925	W	aromatics	1,130	M	aliphatic ethers, phthalates
	845-800	M		1,080, 1,020	W	aromatic overtones
	780-720	S		800, 750	S	aromatic substitution
				1,325, 1,240, 920	weak peaks	

(continued)

TABLE F-3 (continued)

	A			B		
LC5	3,400 (broad)	W	OH, NH	3,500-3,300	W	OH, alcoholic
	3,050	W	unsaturated CH	3,100-3,000	W	CH, aromatic
	2,850, 2,920	W	saturated CH	3,000-2,800	W	CH, aliphatic
	2,220	W	-C≡N	2,215	M	-C≡N, nitrile
	1,700	M	acid, ketones	750	S	C-Cℓ or γ(CH), aromatic rings
	1,600	M	ring vibrations	1,695, 1,595 1,450		minor absorption maxima
	1,050	VS (broad)	Si-O-, ethers			
	750	M	subs. arom., C-Cℓ, fused rings			
LC6	3,400	M (broad)	OH, NH	3,600-2,200	M	OH, acidic
	3,050	W	unsaturated CH	3,100-3,000	M	CH, aromatic
	2,850, 2,920	M	saturated CH	3,000-2,800	M	CH, aliphatic
	1,710	S	acid, ketones	1,709	S	C=O, acidic
	1,680	M	monosubs. amide, ketones	1,600, 1,500	M	C=C, aromatic
	1,600	M	ring vibrations	750-680	S-M	C-Cℓ or γ(CH), aromatic rings
	1,450	M	CH_2	1,235		minor absorption maximum
	1,060	S (broad)	Si-O-, ether			
	740	M	subs. pyridine, C-Cℓ			

(continued)

TABLE F-3 (continued)

	C			D		
LC5	3,335	M	OH or NH	3,400	M	-OH
	3,030	M	aromatics	2,960, 2,920	M	aliphatic CH
	2,960	S	C-H stretch	2,850	W	aliphatic CH
	1,725	S	C=0, esters	1,715	S	carbonyls
	1,680	M	C=0, acids, ketone, aldehyde	1,600	W	amides, amines, aromatic ring
	1,625	M		1,450	W	aliphatics
	1,600	S	aromatics	1,260	W	aromatic ethers, aromatic alcohols, esters
	1,540	W		1,120	W	aromatic overtones, aliphatic ethers
	1,450	S	$C(CH_3)_x$	840, 800, 740, 700	W	aromatic substitution
	1,305-1,280, 1,250-1,190	W	aldehyde, ketone, nitro compounds, arylamine			
	1,135, 1,075	W				
	825, 815	W	aromatics			
	740	S				
	700	M				
LC6	3,450-3,335	W	N-H or O-H	3,300	M	Broad, -OH, -NH
	3,030	W	aromatic	2,960, 2,920, 2,850	M	aliphatic CH
	2,960	M	C-H stretch	1,710, 1,725sh	S	carbonyls
	1,725	S	C=0, esters	1,600	M	benzene ring, amines, heterocyclic N
	1,665	W	C=0, aldehyde, ketones	1,450	M	aliphatics
	1,600	S	aromatics	740, 720, 700	M	aromatic substitution, amines
	1,460	S	$C(CH_3)_x$	1,275br		weak peak

(continued)

TABLE F-3 (continued)

	C			D
LC6	1,335	M	aldehyde	
	1,305	S	aldehyde, ketone,	
	1,280	S	phenyl amines	
	1,250-1,110	W	aromatics	
	770-740			

(continued)

TABLE F-3 (continued)

	A			B		
LC7	3,400	S(br)	OH, NH	3,600-3,200	M	OH, acidic
	2,920	W	saturated CH	3,100-3,000	M	CH, aromatic
	1,620	M	C=C	3,000-2,800	S	CH, aliphatic
				1,710	S	C=0, aliphatic
	Spectrum similar to blank #7.			1,600, 1,500	M	C=C, aromatic
				800-700	M	T(CH), aromatic rings
				1,280		minor absorption maximum
LC8	3,400	S(br)	OH, NH	Not reported		
	1,630	M	C=C			
	1,400	M				
	Spectrum similar to blank #7.					

(continued)

TABLE F-3 (continued)

	C			D		
LC7	4,000	S	H_2O	No IR bands		
	2,960	M	C-H stretch			
	1,640	S	H_2O			
	1,410	M				
	1,250	M	C-O stretch			
	1,110	M				
	1,085-1,065	M	Aromatics			
	770-715	W				
LC 8	3,335	W	OH or NH	3,400	S (broad)	-OH, -NH
	3,225	W	N-H or OH	1,630	W	carboxylates
	3,075	W	aromatics			
	2,960	W	C-H stretch			
	1,725	W	C=O			
	1,650-1,560	W	aromatics			
	1,470-1,380	W	$C(CH_3)_3$			
	1,290-1,250	W	C-O stretch			
	1,190, 1,125, 1,085, 870, 770-750, 715-690	W	aromatics			

APPENDIX G

LRMS RESULTS: CATEGORIES IDENTIFIED IN PHASE II SAMPLES

TABLE G-1. LRMS RESULTS: CATEGORIES IDENTIFIED IN ARTIFICIAL SAMPLE IN CH_2CL_2, ALIQUOT 1

	Categories	Lab A	Lab B	Lab C	Lab D
LC1	Aliphatic hydrocarbons	100	100	NR	NR
LC2	Aliphatic hydrocarbons	10	100	NR	10
	Halogenated aromatic hydrocarbons	100	—		—
	Fused alternate, nonalternate HC's				
	MW <216	100	—		100
	MW >216	10	—		
	Heterocyclic sulfur compounds	100	—		—
	Esters, phthalates	—	—		Trace
LC3	Aromatic hydrocarbons	100		NR	NR
	Benzene, substituted benzenes		100		
	Fused alternate, nonalternate HC's				
	MW <216	100	100		
	MW >216	100	100		
	Heterocyclic sulfur compounds	100	—		
LC4	Aromatic hydrocarbons	100	—	NR	NR
	Nitro aromatic hydrocarbons	—	10		
	Fused alternate, nonalternate HC's				
	MW <216	—	100		
	MW >216	100	100		
	Heterocyclic nitrogen compounds	100	—		
	Heterocyclic sulfur compounds	100	—		
	Esters	10	—		
	Carboxylic acids and derivatives	—	10		

(continued)

TABLE G-1 (continued)

	Categories	Lab A	Lab B	Lab C	Lab D
LC5	Aromatic hydrocarbons	100	—	NR	NR
	Nitro aromatic hydrocarbons	—	100		
	Fused alternate, nonalternate HC's				
	MW <216	—	10		
	MW >216	1	10		
	Esters	1	—		
	Carboxylic acids and derivatives	1	10		
LC6	Aromatic hydrocarbons (substituted)	—	—	10	—
	Nitro aromatic hydrocarbons	—	100	—	—
	Ethers	10	—	—	—
	Phenols	10	10	—	—
	Esters	100	—	100	—
	Heterocyclic nitrogen compounds	100	—	—	—
	Sulfonic acids, sulfoxides	100	—	—	10
	Carboxylic acids and derivatives	100	100	10	100
LC7	Ethers	1	—	NR	NR
	Phenols	10	—		
	Heterocyclic nitrogen compounds	1	—		
	Sulfonic acids, sulfoxides	1	—		
	Carboxylic acids and derivatives	1	100		

(continued)

TABLE G-1 (continued)

	Categories	Lab A	Lab B	Lab C	Lab D
LC8	Ethers	10	—	NR	NR
	Phenols	10	—		
	Esters	1	—		
	Heterocyclic nitrogen compounds	1	—		
	Carboxylic acids	1	100		
	Inorganics	1	—		

TABLE G-2. LRMS RESULTS: CATEGORIES IDENTIFIED IN ARTIFICIAL SAMPLE ON FLYASH MATRIX, ALIQUOT 1

	Categories	Lab A	Lab B	Lab C	Lab D
LC1	Aliphatic hydrocarbons	100	—	NR	100
	Halogenated aliphatics	—	100		—
	Aromatic hydrocarbons	—	—		1
	Halogenated aromatic hydrocarbons	10	100		100
	Sulfur	1	—		—
LC2	Aromatic hydrocarbons	100	—	NR	100
	Halogenated aromatic hydrocarbons	—	100		—
	Fused alternate, nonalternate HC's	—	—		10
LC3	Aromatic hydrocarbons	100		NR	10
	Benzenes, substituted benzenes		100		
	Fused alternate, nonalternate HC's				
	MW <216	100	100		—
	MW >216	100	100		—
	Heterocyclic nitrogen compounds	10	100		10
	Sulfur	1	—		—
LC4	Aromatic hydrocarbons	10		NR	100
	Benzene, substituted benzenes		100		
	Fused alternate, nonalternate HC's				
	MW <216	—	100		—
	Ketones	10	—		—
	Heterocyclic oxygen compounds	—	—		10
	Heterocyclic nitrogen compounds	100	100		10

(continued)

TABLE G-2 (continued)

	Categories	Lab A	Lab B	Lab C	Lab D
LC4 (cont'd)	Heterocyclic sulfur compounds	10	—		10
	Esters	100	—		—
	Sulfur	1	—		—
	Unclassified	100	—		—
LC5	Aromatic hydrocarbons	10	—	NR	—
	Fused alternate, nonalternate HC's MW <216	—	100		—
	Phenols	10	—		10
	Amines	—	—		100
	Heterocyclic nitrogen compounds	100	100		10
	Heterocyclic sulfur compounds	1	—		—
	Esters	10	—		
	Carboxylic acids and derivatives	—	100		100
LC6	Halogenated aromatic hydrocarbons	1	—	NR	—
	Fused alternate, nonalternate HC's MW 216	—	100		—
	Alcohols	—	—		100
	Phenols	100	100		—
	Nitrophenols	—	100		—
	Amines	100	—		100
	Heterocyclic nitrogen compounds	10	100		—
	Heterocyclic sulfur compounds	—	—		100
	Amides	100	—		10
	Carboxylic acids and derivatives	—	100		10

(continued)

TABLE G-2 (continued)

	Categories	Lab A	Lab B	Lab C	Lab D
LC7	Fused alternate, nonalternate HC's MW <216	—	100	NR	—
	Alcohols	—	—		100
	Phenols	10	—		—
	Nitrophenols	—	100		—
	Esters	10	—		—
	Amines	10	—		—
	Heterocyclic nitrogen compounds	10	100		—
	Amides	10	—		—
	Carboxylic acids and derivatives	—	100		—
LC8	Phenols	10	—	NR	—
	Esters	1	—		—
	Heterocyclic nitrogen compounds	1	100		—
	Carboxylic acids and derivatives	—	100		100
	Inorganics	10	—		—

TABLE G-3. LRMS RESULTS: CATEGORIES IDENTIFIED IN FIELD SAMPLE, XAD-2 EXTRACT, RUN 1

	Categories	Lab A	Lab B	Lab C	Lab D
LC 1	Aliphatic hydrocarbons	1	—	NR	NR
	Sulfur	100	100		
LC 2	Aliphatic hydrocarbons	—	—	10	1
	Benzene, substituted benzenes	—	100	—	—
	Fused alternate, nonalternate HC's				
	MW <216	100	100	100	100
	MW >216	10	10		
	Esters, phthalates	—	—	—	1
	Heterocyclic nitrogen compounds	—	10	—	—
	Heterocyclic sulfur compounds	10	—	—	—
LC3	Aliphatic hydrocarbons	—	—	10	—
	Benzene, substituted benzenes	—	100	—	—
	Fused alternate, nonalternate HC's				
	MW <216	100	100	100	100
	MW >216	100	100		
	Heterocyclic sulfur compounds	10	—	—	—
LC4	Benzene, substituted benzenes	—	100	NR	NR
	Fused alternate, nonalternate HC's				
	MW <216	10	100		
	MW >216	10	100		
	Heterocyclic nitrogen compounds	100	10		

(continued)

TABLE G-3 (continued)

	Categories	Lab A	Lab B	Lab C	Lab D
LC5	Benzene, substituted benzenes	—	100	NR	NR
	Fused alternate, nonalternate HC's				
	MW <216	10	100		
	MW >216	—	100		
	Ketones	100	—		
	Nitriles	—	100		
	Heterocyclic nitrogen compounds	100	100		
LC6	Benzene, substituted benzenes	—	100	NR	—
	Fused alternate, nonalternate HC's				
	MW <216	—	100		—
	Ketones	100	—		10
	Nitriles	—	100		—
	Phenols	10	—		—
	Esters, phthalates	10	—		1
	Heterocyclic nitrogen compounds	100	100		100
	Carboxylic acids	10	—		—
LC7	Benzenes, substituted benzenes	—	100	NR	NR
	Fused alternate, nonalternate HC's				
	MW <216	—	100		
	Ketones	1	—		
	Nitriles	—	100		
	Esters	10	—		
	Heterocyclic nitrogen compounds	100	100		
	Carboxylic acids	10	100		

(continued)

TABLE G-3 (continued)

	Categories	Lab A	Lab B	Lab C	Lab D
LC8	Benzene, substituted benzenes	—	100	NR	—
	Fused alternate, nonalternate HC's				
	MW <216	—	100		—
	MW >216	—	100		—
	Ethers	1	—		—
	Phenols	10	—		—
	Esters	1	—		—
	Heterocyclic nitrogen compounds	1	—		—
	Carboxylic acids	1	—		100
	Iron	—	10		—

APPENDIX H

ADDITIONAL ANALYTICAL RESULTS
FROM LAB C

1. TOTAL SAMPLE INFRARED SPECTRA
2. LRMS DATA

TABLE H-1. RESULTS OF INFRARED SPECTROMETRIC ANALYSIS

Sample identification	Band location, cm^{-1}	Band intensity	Band identification
Artificial sample in methylene chloride, aliquot 1	3040	W	C-H stretch aromatic
	2920,2850	S	C-H stretch aliphatic
	1730	S	C=O (esters)
	1610	W	Benzene ring
	1540	S	NO_2 antisym stretch
	1500	W	Benzene ring
	1470	M	CH_2
	1350	S	NO_2 sym stretch
	1280	M	C-O-C stretch
	1270	S	C-O-C stretch (poss. Si-CH_3)
	1240,1220, 1175,1160	W	Unassigned
	1090	S	Prob. benzene ring substitution overlaying Si-O-Si or Si-O-C
	1070	S	
	1045	S	
	1020	S	
	950,930, 920,870, 865,860, 790	W	Benzene ring substitution (poss Si-CH_3 at 790)
	820	S	
	810	S	
	760,750, 740	M	
	710	W	

(continued)

TABLE H-1 (continued)

Sample identification	Band location, cm^{-1}	Band intensity	Band identification
Artificial sample on flyash matrix, aliquot 1	3420	W	OH or NH
	3060,3020	W	C-H stretch aromatic
	2920,2860	S	C-H stretch aliphatic
	1950,1880, 1810	W	Benzene ring overtones
	1730	W	C=O (esters)
	1690	W	C=O (aldehydes/ketones or carboxylic acids)
	1605	S	Benzene ring
	1500	S	Benzene ring
	1460	S	CH_2
	1370	M	CH_3
	1350	W	CH_3
	1300-1150	W	Benzene ring overtones
	1070	W	
	1035	M	
	970	W	
	950	W	
	920	W	
	850	W	
	820	W	
	760	S	
	700	S	

(continued)

TABLE H-1 (continued)

Sample identification	Band location, cm^{-1}	Band intensity	Band identification
Field sample,	3420	W	C=O overtone
XAD-2 extract,	3050	S	C-H stretch aromatic
run 1	2940,2920	S	C-H stretch aliphatic
	2860	W	
	2400,2300	W	Carboxylic acid
	1930	W	Benzene ring
	1720	W	C=O (esters)
	1670	W	C=O (aldehydes/ketones)
	1605	S	Benzene ring
	1510	W	
	1500	M	
	1490	W	
	1460	S	CH$_2$
	1445	S	CH$_2$
	1430	W	Carboxylic acid
	1370,1360	W	CH$_3$
	1305	W	S=O antisym stretch
	1270	M	C-O-C stretch
	1250	M	C-O-C stretch
	1190	S	C-O-C stretch
	1140	M	S=O sym stretch
	1100	W	C-O stretch
	1040	M	Benzene ring substitution
	1020	W	
	950	W	
	880	W	
	870	W	
	850	S	
	820	S	
	775	S	
	740	S	
	720	S	

TABLE H-2. ADDITIONAL LRMS RESULTS FROM LAB B AFTER RECALCULATION

Artificial sample in methylene chloride, aliquot 1, LC 3

1. Categories present
    - 100 Fused ring hydrocarbons
    - 10 Aromatic hydrocarbons
2. Subcategories, specific compounds
    - 100 Chrysene (or isomer)
    - 10 Aromatic hydrocarbons
    - 1 Pyrene (or isomer)
3. Other
    - 10 MW = 234 (probably fused ring aromatic)
    - 10 M/e = 279

Artificial sample in methylene chloride, aliquot 1, LC 6

1. Categories present
    - 10 Esters
    - 10 Fused ring hydrocarbons
2. Subcategories, specific compounds
    - 10 Phthalate esters
    - 10 Chrysene (or isomer)
3. Other
    - 1 m/e = 167

XAD-2 extract, run 1, LC 6

1. Categories present
    - 10 Esters
2. Subcategories, specific compounds
    - 10 Phthalate esters
3. Other

APPENDIX I

LRMS RESULTS: SPECIFIC COMPOUNDS IDENTIFIED IN PHASE II SAMPLES

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TABLE I-1. LRMS RESULTS: SPECIFIC COMPOUNDS IDENTIFIED IN ARTIFICIAL SAMPLE IN CH_2CL_2, ALIQUOT 1

	m/e Specific Compound	Lab A	Lab B	Lab C	Lab D
LC1	422 aliphatic hydrocarbon, possibly squalane	100	100	NR	NR
LC2	112 chlorobenzene	100	—	NR	—
	154 acenaphthene/biphenyl	100	—		—
	184 dibenzthiophene	100	—		P (u)
	228 chrysene/benzanthracenes	10	—		100
	234 naphthothianaphthene	10	—		—
	278 dibenzanthracene	—	—		Trace
	422 aliphatic hydrocarbon, possibly squalane	10	100		
LC3	154 acenaphthene/biphenyl	100	100	NR	NR
	167 unidentified				
	184 dibenzthiophene	100	100(u)		
	198 methyldibenzthiophene	1	—		
	202 pyrene/fluoranthene	—	100		
	212 dimethyl/ethyldibenzthiophene	1	—		
	226 benz[ghi]fluoranthene	—	100		
	228 chrysene/benzanthracenes	100	100		
	234 naphtholthianaphthene	10	10(u)		
	279 unidentified				
LC4	152 aminonitrotoluene	10	—	NR	NR
	182 dinitrotoluene	100	10		
	184 dibenzthiophene	100	100(u)		
	202 pyrene/fluoranthene	—	100		
	217 benzocarbazole	100	—		
	222 diethylphthalate	10	—		
	226 benzfluoranthene	—	100		
	228 chrysene/benzanthracenes	100	100		
	234 naphtholthianaphthene	10	10(u)		
	298 methylstearate	—	10		

(continued)

TABLE I-1 (continued)

	m/e Specific Compound	Lab A	Lab B	Lab C	Lab D
LC5	152 aminonitrotoluene	1	—	NR	NR
	182 dinitrotoluene	100	100		
	202 pyrene/fluoranthene	—	10		
	228 chrysene/benzanthracenes	1	10		
	270 methylpalmitate	1	—		
	298 nonadecanoic acid	1			
	298 methylstearate		10		
LC6	94 phenol	100	10	(phthalate esters; aromatic substituted compounds)	(aliphatic carboxylic acid, C_{17}-C_{18}; dimethoxybenzoic acid)
	108 cresol	10	—		
	129 quinoline	100	—		
	182 dinitrotoluene	—	100		
	214 dimethoxybiphenyl	10	100(u)		
	222 diethylphthalate	100	10		
	230 ditolylsulfoxide	100	100(u)		
	256 palmitic acid	100	100		
	270 methylpalmitate	10	—		
	284 stearic acid	10	100		
	316 unidentified	1(u)	—		
	355 unidentified	1(u)	—		
	370 unidentified	1(u)	—		
LC7	129 quinoline	1	—	NR	NR
	186 biphenol/phenoxyphenol	10	—		
	214 dimethoxybiphenyl	1	100(u)		
	230 ditolylsulfoxide	1	100(u)		
	256 palmitic acid	1	100		
	262 unidentified	1(u)	—		
	284 stearic acid	—	100		

(continued)

TABLE I-1 (continued)

	m/e Specific Compound	Lab A	Lab B	Lab C	Lab D
LC8	129 quinoline	1	—	NR	NR
	134 zinc chloride	1	—		
	182 unidentified	—	10(u)		
	186 biphenol/phenoxyphenol	10	—		
	214 methoxybiphenyl	10	10(u)		
	230 unidentified	—	10(u)		
	256 palmitic acid	1	—		
	270 methylpalmitate	1	—		
	298 nonadecanoic acid	1			
	298 methylstearate		100		
	phthalate, not specifically identified	1	—		

P = present but not quantified.

u = peak at indicated m/e unidentified.

TABLE I-2. LRMS RESULTS: SPECIFIC COMPOUNDS IDENTIFIED IN ARTIFICIAL SAMPLE ON FLYASH MATRIX, ALIQUOT 1

	m/e	Specific Compound	Lab A	Lab B	Lab C	Lab D
LC1	77, 91, 105	benzene, alkyl series	—	—	NR	1
	128-156	naphthalene, alkyl series	—	—		1
	240-560	alkanes	100	—		100
	256	sulfur	1	—		—
	258	hexachlorobutadiene	—	100		—
	282	hexachlorobenzene	10	100		10
	332	hexachloronaphthalene	1	—		—
	>300	unidentified chlorinated compounds	1	10		—
	400	octachloropentafulvalene	—	100		—
		Alkene and cyclic alkene and diene	—	—		100
		Alkyne and cycloalkene, terpenes	—	—		100
LC2	106-148	alkylbenzenes	100	—	NR	—
	119	benzotriazole	—	—		P
	178-206	phenanthrene/anthracene, alkyl series	—	—		10
	180-208	stilbene, alkyl series	—	—		10
	192, 206, 220, 236	naphthalene, naphtheno-substituted	—	—		100
	220-330	alkylated aromatic hydrocarbons	100	—		—
	200-400	alkylated aromatic hydrocarbons	10	—		—
	284, 286	hexachlorobenzene	—	—		P
	290-400	chlorinated material	1	—		—
	400	octachloropentafulvalene	—	100		—
	>400	polyhalogenated compounds	—	10		—

(continued)

TABLE I-2 (continued)

	m/e Specific Compound	Lab A	Lab B	Lab C	Lab D
LC3	92, 106, 122 benzene, alkyl series	—	—	NR	100
	104, 208 styrene and styrene dimer	100	—		—
	117 indole	—	—		10
	118 methylstyrene	100	—		—
	128 naphthalene/azulene	1	100		—
	129 quinoline	1	—		10
	130 divinylbenzene	10	—		—
	142 methylnaphthalene	1	—		—
	152 acenaphthylene/biphenylene	—	100		—
	155 phenylpyridine	—	100		—
	167 carbazole	—	100		—
	178 phenanthrene/anthracene	100	100		—
	180 stilbene	100	100		—
	181 styrylpyridine/methyl carbazole	10	100		P(u)
	180, 206, 208 partially saturated aromatics	—	100		
	180, 192, 194, 206, 208 alkyl substituted aromatic series	—	100		—
	182 dimethylbiphenyl	—	100		—
	192 methylanthracene/phenanthrene	100	—		—
	192 sulfur	1	—		—
	193 methyl acridine	10	—		P(u)
	193 methylbenzoquinoline, naphthaquinaldine, or phenylindole	—	100		—
	194 methyl stilbene	100	—		—
	194 phenylbenzimidazole	—	100		—
	202 fluoranthene/pyrene	—	100		—
	204 dibenzoheptafulvalene	—	100		—
	206 diphenylbutadiene	—	100		—
	207 methylphenylindole	—	100		P(u)
	208 diphenylbutene	—	100		—
	210 benzil/ditolylethane/alkyl carbazole	—	100		—
	217 benzocarbazole	10	—		—
	226 benzfluoranthene	—	100		—

(continued)

TABLE I-2 (continued)

	m/e	Specific Compound	Lab A	Lab B	Lab C	Lab D
LC3 (cont'd)	232	unidentified sulfur containing material	1	—		—
	234	hexahydrobenzanthracene	—	100(u)		—
	236	unidentified	—	100(u)		—
	200-400	alkylated polycyclic material	100	—		—
	309	unidentified	—	—		P(u)
	>400	polyhalogenated material	1	10		—
	180 (452)	phenazine or phenanthroline (halogenated)	—	100		—
LC4	104, 208	styrene/styrene dimer	10	—	NR	None Identified
	117, 193, 207	indole and aryl and alkyl substituted indole	100	100		
	129, 193	quinoline and aryl and alkyl substituted quinolines	—	100		
	136	methyl benzoate	100	—		
	152	acenaphthylene/biphenylene	—	100		
	167, 181, 210	carbazole and alkyl substituted carbazoles	10	100		
	178	phenanthrene/anthracene	10	100		
	179	acridine	10	—		
	180	stilbene	10	100		
	180, 192, 194, 206, 208	partially substituted aromatics; alkyl substituted aromatic series	—	100		
	180 (452)	phenazine/phenanthroline (halogenated)	—	100		
	182	dimethylbiphenyl	—	100		
	192	sulfur	1	—		
	193	methylacridine	10	—		

(continued)

TABLE I-2 (continued)

	m/e	Specific Compound	Lab A	Lab B	Lab C	Lab D
LC4 (cont'd)	194	methylstilbene	10			
	194	phenylbenzimidazole		100		
	195	dimethylcarbazole	10	—		
	200	phenothioxine	10	—		
	202	fluoranthene/pyrene	—	100		
	204	dibenzoheptofulvaline	100(u)	100		
	206	diphenylbutadiene	—	100		
	208	diphenylbutene	—	100		
	242, 270	unidentified	100(u)	—		
	119, 240	unidentified	100(u)	—		
	200-400	polycyclics	1	—		
	232	probable sulfur species	1	—		
LC5	84	thiophene/methylene chloride	—	—	NR	P
	94	phenol	—	—		10
	104, 208	styrene/styrene dimer	10	—		—
	117	indole	100	100		—
	121	benzamide	—	100		
	121	aniline				100
	129, 193	quinoline and aryl and alkyl substituted quinoline	1	100		10
	135	toluamide	—	100		—
	136	methylbenzoate	10	—		—
	155	unidentified	—	—		P(u)
	178	anthracene/phenanthrene	—	100		—
	180	stilbene	1	—		—
	181	methyl carbazole	1	100		—
	182	unidentified	—	100(u)		—
	193	phenylindole	10	100		—
	193	naphthoquinaldine		100		

(continued)

TABLE I-2 (continued)

	m/e	Specific Compounds	Lab A	Lab B	Lab C	Lab D
LC5 (cont'd)	194	methylstilbene	1	—		—
	207	substituted indole	—	100		—
	217	benzocarbazole	10	—		—
	225	dibenzamide	—	100		—
	236	diphenylthiophene	1	—		—
	246	diphenylphenol	10	—		—
	130, 240, 242	unidentified	1(u)	—		—
	>400	polyhalogenated compounds	—	10		—
		Hydrazines	—	—		100
		Long chain unsaturated acid or ester	—	—		100
LC6	93	aniline	100	—	NR	None Identified
	94	phenol	100	10		
	108	cresol	10	10		
	118	methylstyrene	10	—		
	121	benzamide	100	100		
	129	quinoline	10	100		
	130	methylindene	—	100		
	135	toluamide	—	100		
	139	nitrophenol	10	100		
	178	anthracene/phenanthrene	—	100		
	181	methylcarbazole	—	100		
	182	unidentified	—	100(u)		
	193	phenylindole/naphthaquinaldine	10	100		
	199	phenathiazine	—	100		
	207	methylphenylindole	10	100		
	213	unidentified	—	100(u)		
	248	Cl_3 species	1	—		
	282	hexachlorobenzene	1	—		
		Sulfate decomposition, SO_2^+, SO_3^+	1	—		

(continued)

TABLE I-2 (continued)

	m/e	Specific Compounds	Lab A	Lab B	Lab C	Lab D
LC7	93	aniline	10	—	NR	
	104	unidentified	—	10(u)		
	121	benzamide	10	100		
	130	methylindene	—	10		
	135	toluamide	—	100		
	139	nitrophenol	10	100		
	178	anthracene/phenanthrene	—	100		
	181	methylcarbazole	10(u)	100		
	182	unidentified	—	100(u)		
	193	methylbenzoquinoline, naphthoquinaldine, or phenylindole	10	100		
	199	phenothiazine	—	100		
	207	methylphenylindole	10	100		
	213	unidentified	—	100(u)		
	223	unidentified	10(u)	100(u)		
	237	unidentified	10(u)	—		P(u)
	240	unidentified	10(u)	—		
	263	unidentified	10(u)	—		
	281	unidentified	—	—		P(u)
		Phthalate, not identifiable	10	—		
LC8	44	carbon dioxide	10	—	NR	None Identified
	104	unidentified	—	10(u)		
	121	benzamide	—	10		
	129	quinoline	1	100		
	134	zinc chloride	10	—		
	135	toluamide	—	100		
	163	unidentified	1	—		
	181	methylcarbazole	—	100		
	182	unidentified	—	100(u)		
	186	biphenol/phenoxyphenol	10	—		
	193	aryl substituted quinoline	—	100		
	199	phenothiazine	—	100		
	207	methylphenylindole	—	100		
		phthalate, not identifiable	1	—		

P = present but not quantified.
u = peak at indicated m/e unidentified.

TABLE I-3. LRMS RESULTS: SPECIFIC COMPOUNDS IDENTIFIED IN FIELD SAMPLE, XAD-2 EXTRACT, RUN 1

	Specific Compounds		Lab A	Lab B	Lab C	Lab D
LC1	240-380	alkanes	1	—	NR	NR
	256	sulfur	100	100		
LC2	128-170	azulene/naphthalenes	10	10	—	—
	142	methylnaphthalene	—	10	—	—
	152	acenaphthylene/biphenylene	10	100	—	100
	153	unidentified	—	100(u)	—	—
	154	biphenyl/acenaphthene	10	100	—	—
	167	carbazole	—	10	—	—
	178	anthracene/phenanthrene	100	100	—	100
	184	dibenzthiophene	10	—	—	—
	192	methylanthracene/phenanthrene	100	—	—	—
	202	pyrene	100	100	100	100
	216	benzofluorene/methylpyrene	10	100	—	100
	230	terphenyl	—	10	—	—
	182, 196, 220	unidentified PAH	10	—	—	—
	228-242	chrysene (isomers)	—	—	—	100
	242-268	benzo(a)pyrene (isomers)	—	—	—	100
	278	benzochrysene	—	—	—	10
	200-300	unidentified polycyclics	1(u)	—	—	—
		Ester, phthalate	—	—	—	1
		Benzanthracene	—	—	100	—
		Hydrocarbons	—	—	10	1
LC3	128-170	naphthalene/alkyl naphthalene	100	10	—	—
	152	acenaphthylene/biphenylene	—	100	—	—
	154	acenaphthene/biphenyl	100	100	—	—
	166	methylacenaphthylene	10	—	—	—
	168	methylbiphenyl	—	100	—	—
	178	anthracene/phenanthrene	100	100	—	10

(continued)

TABLE I-3 (continued)

	Specific Compounds		Lab A	Lab B	Lab C	Lab D
LC3 (cont'd)	184	dibenzthiophene	10	—	—	—
	192	methylanthracene/phenanthrene	100	100	—	—
	202	pyrene/fluoranthene	100	100	100	100
	216	benzofluorene/methylpyrene	10	100	100	—
	218	benzylnaphthylene	—	100	—	—
	226	benzfluoranthene	—	100	—	—
	228	chrysene/benzanthracenes	100	100	100	100
	252	benzpyrenes, etc.	10	—	10	10
	276	benzoperylene, etc.	10	10	—	—
	278	dibenzanthracenes, etc.	10	10	10	10
	302	dibenzpyrene, etc.	10	—	—	—
	200-300	unidentified PAH	10(u)	—	—	—
	343, 357, 371	unidentified	1(u)	—	—	—
LC4	167	carbazole	100	10	NR	NR
	178	anthracene/phenanthrene	10	100		
	180	phenazine/phenanthroline	10	—		
	181	methyl carbazole	10	—		
	195	dimethyl carbazole	10	—		
	202	pyrene/fluoranthene	10	100		
	216	benzofluorene/methylpyrene	—	100		
	217	benzocarbazole	10	—		
	226	benzfluoranthene	—	100		
	228	chrysene, triphenylene, etc.	—	100		
	252	perylene, benzpyrene, benzfluoranthene	10	10		
	267	dibenzocarbazole	10	—		
	276	benzoperylene, etc.	10	10		
	278	picene/benzchrysene	—	10		
	200-280	unidentified polycyclics	10	—		
	200-400	unidentified polycyclics	1	—		

(continued)

TABLE I-3 (continued)

	Specific Compounds		Lab A	Lab B	Lab C	Lab D
LC5	152	acenaphthylene/biphenylene	—	100	NR	NR
	153	naphthoisocyanid/β-naphthonitrile	100	100		
	154	acenaphthene/biphenyl	—	100		
	167	carbazole	10	10		
	178	anthracene/phenanthrene	10	100		
	179	acridine	10	—		
	192	methylanthracene/phenanthrene	—	100		
	193	methylacridine	10	—		
	194	unidentified	10(u)	100(u)		
	202	pyrene/fluoranthene	—	100		
	203	cyanoanthracene	10(u)	100		
	217	benzocarbazole	10	—		
	220	diphenylimidazole/ diphenylpyrazole	10(u)	100		
	228	chrysene, triphenylene, etc.	—	100		
	230	benzanthrone	100	—		
	244	methylbenzanthrone	10	100(u)		
	280	dibenzofluorenone	10	10(u)		
	191, 234, 270	unidentified	10(u)	—		
	200-400	unidentified	1(u)	—		
LC6	94	phenol	10	—	NR	—
	108	cresol	10	—		—
	122	benzoic acids	10	—		—
	152	acenaphthylene/biphenylene	—	100		—
	153	beta-naphthonitrile	—	100		—
	154	acenaphthene/biphenyl	—	100		—
	167	carbazole	10	100		100
	168	methylbiphenyl	—	100		—
	179	acridine	100	—		100

(continued)

TABLE I-3 (continued)

	Specific Compounds		Lab A	Lab B	Lab C	Lab D
LC6 (cont'd)	180	fluorenone, dihydroanthracene, dihydrophenanthrene	100	100		—
	193	methylacridine, phenylindole, methylbenzoquinoline, β-naphthoquinaldine	10	100		—
	194	methylfluorenone	10	—		—
	202	pyrene/fluoranthene	—	100		—
	203	azapyrene	10(u)	—		100
	204	unidentified	10(u)	100(u)		—
	207, 208, 243 253	polycyclic components	10(u)	—		—
	220	diphenylimidazole/ diphenylpyrazole	—	100		—
	229	anthraquinoline	10	—		—
	230	benzanthrone/terphenyl	10	100		10
	244	methylbenzanthrone	10	—		—
	278	dibutylphthalate/dibenzo-acridine	10	—		100
	280	dibenzofluorenone	10	10(u)		—
	200-350	unidentified	1(u)	—		—
LC7	122	benzoic acid	10	10	NR	NR
	129	quinoline	100	100		
	143	methylquinoline	100	—		
	152	acenaphthylene/biphenylene	—	100		
	153	beta-naphthonitrile	—	100		
	154	acenaphthene/biphenyl	—	100		
	167	carbazole	1	100		
	178	phenanthrene/anthracene	—	10		
	179	acridine	100	—		
	192	methylphenanthrene/anthracene	—	100		

(continued)

TABLE I-3 (continued)

	Specific Compounds		Lab A	Lab B	Lab C	Lab D
LC7 (cont'd)	193	methylacridine/phenylindole/ beta-naphthoquinaldine	10	100	NR	NR
	202	pyrene/fluoranthene	—	100		
	203	cyano-anthracene	100	100		
	217	benzocarbazole	1	—		
	229	anthraquinoline	1	—		
	230	benzanthrone/terphenyl	1	100		
	390	dioctylphthalate	10	—		
LC8	122	benzoic acid	1	—	NR	—
	126	$FeCl_2$	—	10		—
	129	quinoline	1	—		—
	157	dimethylquinoline	1	—		—
	178	phenanthrene/anthracene	—	100		—
	186	biphenol/phenoxyphenol	10	—		—
	202	pyrene/fluoranthene	—	100		—
	214	dimethoxybiphenyl	1	—		—
	228	chrysenes, etc.	—	100		—
	278	unsaturated carboxylic acid	—	—		P
	322	Fe_2Cl_6	—	10		—
	390	dioctylphthalate	1	—		—

u = peak at indicated m/e unidentified.
P = present but not quantified.